**AL-PINNs: Augmented Lagrangian relaxation method for Physics-Informed Neural Networks**

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**Abstract**

Physics-Informed Neural Networks (PINNs) has become a prominent application of deep learning in scientific computation, as it is a powerful approximator of solutions to nonlinear partial differential equations (PDEs). There have been numerous attempts to facilitate the training process of PINNs by adjusting the weight of each component of the loss function, called adaptive loss balancing algorithms. In this paper, we propose an Augmented Lagrangian relaxation method for PINNs (AL-PINNs). We treat the initial and boundary conditions as constraints for the optimization problem of the PDE residual. By employing Augmented Lagrangian relaxation, the constrained optimization problem becomes a sequential minimax problem so that the learnable parameters \(\lambda\)'s adaptively balance each loss component. Our theoretical analysis reveals that the sequence of minimizers of the proposed loss functions converges to an actual solution for the Helmholtz, viscous Burgers, and Klein–Gordon equations. We demonstrate through various numerical experiments that AL-PINNs yields a much smaller relative error compared with that of state-of-the-art adaptive loss balancing algorithms.

**1. Introduction**

Starting from a seminal work given in Raissi et al. (2019), Physics-Informed Neural Networks (PINNs) has become a significant research interest in many scientific disciplines, along with the great development of deep learning. Due to its simple and easy-to-implement algorithm and powerful approximation capacity, numerous successful applications of PINNs have been reported in the last decade (Lu et al., 2021a). We refer the readers to a recent review by Karniadakis et al. (2021) for more information.

There are several branches of theoretical convergence results for PINNs. For example, Shin et al. (2020) have shown that the neural network converges to a classical solution for the linear second-order elliptic and parabolic equations. Another branch of studies, including Sirignano & Spiliopoulos (2018), Jo et al. (2020), Hwang et al. (2020) analyzed continuous loss functions and proved that an actual error can be bounded by a continuous function of each loss component (e.g., (5)). However, the precise functional form of such an upper bound, as well as the best loss function to approximate solutions of given PDEs, remain to be discovered.

Recently, there has been a considerable effort to find the best surrogate loss function by manipulating the ratio of each loss component to form a loss function, using loss balancing algorithms (see Section 1.1). However, most current approaches are limited to individual empirical observations which may have a detrimental effect on training PINNs. We propose a more universal approach by setting the initial and boundary conditions as constraints for the optimization problem. We solve such a constrained optimization problem involving a neural network with the augmented Lagrangian method.

The augmented Lagrangian relaxation method has been successfully applied throughout constrained deep learning literature (see Section 1.1). For the problems involving PDEs, the constrained optimization methods are intensively studied using the Deep Ritz Method (DRM) due to their constrained nature. For example, the convergence of the penalty method for the DRM is given by Müller & Zeinbohner (2019), and a deep augmented Lagrangian method for the DRM is proposed by Huang et al. (2021). However, the convergence of the augmented Lagrangian method has never been discovered for either PINNs or the DRM. To the best of our knowledge, this is the first attempt to show the convergence of the augmented Lagrangian method for PINNs.

In this paper, we propose the Augmented Lagrangian relaxation method for training PINNs (AL-PINNs) to facilitate the training of PINNs. Considering the initial and bound-
ary conditions as constraints, we reformulate the training of PINNs into a constrained optimization problem. Using the augmented Lagrangian relaxation method, we derive a novel sequence of loss functions with adaptively balanced loss components. In Section 3, we prove that the minimizers of the loss functions converge to an actual solution. In Section 4, we first detail experiments exhibiting the advantages of the augmented Lagrangian relaxation compared with the penalty, and Lagrange multiplier methods. We then provide experimental results that demonstrate the outstanding performance of the proposed AL-PINNs compared with several adaptive loss balancing algorithms using the Helmholtz, viscous Burgers, and Klein–Gordon equations. Therefore, the proposed AL-PINNs is a convergence guaranteed universal framework that uniformly outperforms other loss balancing algorithms in solving PDEs.

1.1. Related works

Constrained Deep Learning. Imposing hard constraints on the output of an artificial neural network is a challenging problem. Marquez-Neila et al. (2017) discussed the possibility of imposing hard constraints on the output of a neural network in a computationally feasible way by using the Krylov subspace method. However, they also claimed that the performance of the proposed method is not superior to that of the soft constrained one. On the other hand, from a soft constraint perspective, the Augmented Lagrangian method (ALM), or equivalently, Lagrangian dual formulation, has been widely adopted for solving constrained optimization problems involving neural networks. For instance, Nandwani et al. (2019) demonstrated that constrained formulation with ALM yields state-of-the-art performance in three NLP benchmarks. Sangalli et al. (2021) presented the use of ALM for solving class-imbalanced binary classification, and Fioretto et al. (2020) applied ALM to optimal power flow prediction problems. For problems involving PDEs, Hwang and Son (2021) proposed an ALM approach to impose several physical conservation laws of kinetic PDEs on the neural network and Lu et al. (2021b) proposed PINNs with hard constraints for the inverse design. For an extrapolation problem, Kim et al. (2021) proposed the Dynamic Pooling Method (DPM) to impose a soft constraint on a residual loss function for training PINNs.

Imposing the initial and boundary conditions. The use of initial and boundary conditions as hard constraints is frequently considered in PINNs literature. Several studies proposed to set the boundary conditions as hard constraints by utilizing a distance function $\text{dist}(x, \partial \Omega)$ (see Lagaris et al. 1998; Berg & Nyström 2018; Jo et al. 2020; Son et al. 2021; Sukumar & Srivastava 2021 for examples). However, in most existing studies regarding PDEs and neural networks, the boundary conditions are relaxed into the loss function in a soft manner using a quadratic penalty function (see Sirignano & Spiliopoulos 2018; Raissi et al. 2019; Yu et al. 2017 for examples). For the Deep Ritz Method (DRM), Müller & Zeinhofer (2019) have shown that the sequence of quasi-minimizers for the variational problem with the penalty method converges to a true solution.

Loss balancing algorithms for PINNs. Loss balancing algorithms have been widely studied to deal with various kinds of stability issues in the training dynamics of PINNs. For instance, a non-adaptive weighting strategy that considers the weights as hyperparameters is proposed by Zhao (2020). Adaptively balancing the components of the loss function by using a soft attention mechanism has been considered by McClenny & Braga-Neto (2020) in order to give more weight to the region where the solution exhibits stiff transition. Wang et al. (2021) argued that the numerical stiffness in gradient statistics causes unstable back-propagation, and proposed an adaptive loss balancing algorithm, called learning rate annealing, to address this issue. Wang et al. (2022) observed a discrepancy in the convergence rate of loss components, and proposed to use the eigenvalues of the NTK to balance the convergence rate. Another branch of study considers the training of PINNs as a multi-objective learning where the components compete with each other (see, van der Meer et al. 2020; Bischof & Kraus 2021; Rohrhofer et al. 2021 for more information).

2. Preliminaries and Methods

2.1. Preliminaries

Consider a generic constrained optimization problem on $\mathbb{R}^n$.

\[
\arg \min_{\theta} J(\theta),
\]

subject to $C(\theta) = 0, \theta \in \mathbb{R}^n, C : \mathbb{R}^n \to \mathbb{R}^m$. Constrained optimization problems have been deeply investigated in convex optimization literature (Boyd et al. 2004). A naive approach to solve (1) is to relax the constraints into the objective function via the penalty method; i.e.,

\[
\mathcal{J}_n(\theta) = J(\theta) + \beta_n || C(\theta) ||_2^2,
\]

where $\beta_n \to \infty$. However, this approach exhibits numerical instabilities due to the large values of $\beta_n$ (Bertsekas 1976).

Another method for solving (1) is to consider the Lagrangian duality

\[
\mathcal{J}_\lambda(\theta) = J(\theta) + \langle \lambda, C(\theta) \rangle_{\mathbb{R}^m},
\]

where $\lambda \in \mathbb{R}^m$ and $\langle \cdot, \cdot \rangle_{\mathbb{R}^m}$ denotes the standard inner product on $\mathbb{R}^m$. Since

\[
\min_{C(\theta) = 0} J(\theta) = \min_{C(\theta) = 0} \mathcal{J}_\lambda(\theta) \geq \min_{\theta \in \mathbb{R}^n} \mathcal{J}_\lambda(\theta),
\]
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We consider a general class of PDEs that reads as:

\[ u \]

where \( u \) denotes the neural network solution and \( \theta \) denotes a set of parameters. However, as the penalty method often fails to approximate an accurate solution, adaptive loss balancing algorithms are commonly applied in the literature. As pointed out in previous works, the boundary conditions often cause instability in the training of PINNs and DRM (See, Wang et al., 2021, 2022; Müller & Zeinhofer, 2021, 2019).

In this study, we propose a novel class of loss functions for PINNs based on the augmented Lagrangian method, which aim to solve the following constrained optimization problem:

\[
\begin{align*}
\text{arg min}_{\theta} & \| Nu_{nn}(\theta) - f \|_{L^2(\Omega)}, \\
\text{subject to} & \| Tu_{nn}(\theta) - g \|_{L^2(\partial\Omega)}.
\end{align*}
\] (4)

In the augmented Lagrangian method, the constraint in (4) is relaxed into the objective function via the Lagrange multiplier \( \lambda \in L^2(\partial\Omega) \). The resulting objective function reads as:

\[
\mathcal{L}_\lambda(\theta) = \| Nu_{nn}(\theta) - f \|_{L^2(\Omega)} + \beta \| Tu_{nn}(\theta) - g \|_{L^2(\partial\Omega)} + (\lambda, Tu_{nn}(\theta) - g)_{L^2(\partial\Omega)}
\] (5)

where \((\cdot, \cdot)_{L^2(\partial\Omega)}\) is the standard \(L^2\) inner product.

As in the discussed in the previous subsection, we solve the following max-min problem:

\[
\max_{\lambda \in L^2(\partial\Omega)} \min_{\theta} \mathcal{L}_\lambda(\theta). \quad (6)
\]

We solve the above max-min problem by the gradient descent-ascent algorithm for \( \theta-\lambda \). The update rules are given as:

\[
\theta \leftarrow \theta - \eta_\theta \nabla_\theta \mathcal{L}_\lambda(\theta), \\
\lambda \leftarrow \lambda + \eta_\lambda \nabla_\lambda \mathcal{L}_\lambda(\theta),
\]

where \( \eta_\theta \) and \( \eta_\lambda \) are the predefined learning rates for \( \theta \) and \( \lambda \), respectively.

In the numerical experiments, we treat \( \lambda \) as a discretization; i.e., \( \lambda \approx (\lambda(x_1^b), ..., \lambda(x_{N_b}^b)) \). We discretize the loss function in (5) on uniform grid points. Let \( \{x_1^b, x_2^b, ..., x_{N_b}^b\} \subset \Omega \) and \( \{x_1^b, x_2^b, ..., x_{N_b}^b\} \subset \partial\Omega \) be the uniform grid points. Then, the objective function is discretized into

\[
\mathcal{L}_\lambda(\theta) \approx \sum_{i=1}^{\Omega} (Nu_{nn}(x_i^b; \theta) - f(x_i^b))^2 + \frac{\beta|\partial\Omega|}{N_b} \sum_{j=1}^{N_b} (Tu_{nn}(x_j^b) - g(x_j^b))^2 + \frac{|\partial\Omega|}{N_b} \sum_{j=1}^{N_b} \lambda(x_j^b)(Tu_{nn}(x_j^b) - g(x_j^b))
\]

and the corresponding update rules are given as:

\[
\theta \leftarrow \theta - \eta_\theta \nabla_\theta \mathcal{L}_\lambda(\theta), \\
\lambda_j \leftarrow \lambda_j + \eta_\lambda \nabla_\lambda \mathcal{L}_\lambda(\theta),
\]

where \( \lambda_j = \lambda(x_j^b) \), for \( j = 1, 2, ..., N_b \).

3. Convergence Analysis

In this section, we provide theoretical justifications of the proposed method by showing its convergence to an actual
solution. Proofs of the theorems in this section are provided in Section C.

Consider a generic boundary value problem:

\[ Nu = f, \quad \text{for } x \in \Omega, \]
\[ Tu = g, \quad \text{for } x \in \partial\Omega, \]

where \( N \) and \( T \) denote the differential and trace operator, respectively. In this study, we assume that \( \Omega \) is a bounded, open, and connected subset of \( \mathbb{R}^n \), where \( \partial\Omega \) denotes the boundary of \( \Omega \). If (7) admits a unique strong solution (i.e., the differentiability of the solution is guaranteed as required in \( N \) or \( B \)), then solving (7) is equivalent to finding a minimizer of the following functional:

\[
L(u) = \begin{cases} 
||Nu - f||_{L^2(\Omega)}^2 + (Bu = g) & \text{for } (u \in A_n) \\
\infty & \text{for } (u \notin A_n)
\end{cases}.
\]

In this study, we consider the following sequence of loss functionals \( \{L_n\}_{n=1}^{\infty} \) that incorporates the proposed loss functions in [5].

\[
L_n(u) = \begin{cases} 
||Nu - f||_{L^2(\Omega)}^2 + \beta||Tu - g||_{L^2(\partial\Omega)}^2 + \langle \lambda_n, Tu - g \rangle_{L^2(\partial\Omega)}, & \text{for } (u \in A_n) \\
\infty, & \text{for } (u \notin A_n)
\end{cases}
\]

where \( A_n \) denotes a set of neural networks with width \( n \) and depth \( O(\dim(\Omega)) \). We will show that the sequence of minimizers of the loss functionals \( L_n \) converges to an actual solution. We first introduce the notion of \( \Gamma' \)-convergence of functionals that is at the core of established convergence theory. Modifying Definition 4.1 in Dal Maso (2012), we define the \( \Gamma' \)-convergence as follows.

**Definition 3.1.** Let \( X \) be a topological space and \( \{F_n\}_{n \in \mathbb{N}} : X \rightarrow (-\infty, \infty] \) be a sequence of functionals. Then, \( \{F_n\}_{n \in \mathbb{N}} \) is said to \( \Gamma' \)-converge to \( F \) if \( \forall \epsilon > 0 \), there exists a sequence \( \{x_n\}_{n \in \mathbb{N}} \) of quasi-minimizers of \( F_n \) such that

\[
\lim_{n \rightarrow \infty} F_n(x_n) \leq \liminf_{n \rightarrow \infty} F_n(x_n) + \epsilon.
\]

where \( F_A = \{x \in X | F(x) < \infty\} \) is an admissible set of \( F \).

The following definition describes the equicoercivity of the sequence of functionals.

**Definition 3.2 (Definition 7.6 in Dal Maso (2012)).** Let \( X \) be a topological space and \( \{F_n\}_{n \in \mathbb{N}} : X \rightarrow (-\infty, \infty] \) be a sequence of functionals defined on \( X \). Then, we say that \( \{F_n\}_{n \in \mathbb{N}} \) is equicoercive if \( \forall r \in \mathbb{R} \) and there is a compact set \( K_r \subset X \) such that

\[
\bigcup_{n \in \mathbb{N}} \{x \in X : F_n(x) \leq r\} \subset K_r.
\]

Thus, the compactness argument can be applied to the sequence of minimizers of an equicoercive sequence of functionals. Indeed, the boundedness of minimizers ensures the existence of a convergent subsequence. The following theorem bridges the notion of \( \Gamma' \)-convergence with the convergence of dominant quasi-minimizers of the functionals.

**Theorem 3.3.** Let \( X \) be a reflexive Banach space and \( \{F_n\}_{n \in \mathbb{N}} \) be a sequence of equicoercive functionals on \( X \) that \( \Gamma' \)-converges to \( F \) with a unique minimizer \( x \). Then, every sequence \( \{x_n\}_{n \in \mathbb{N}} \) of quasi-minimizers of \( F_n \) converges weakly to \( x \).

Now, we refer to a lemma which is essential to prove the theorem.

**Lemma 3.4.** Let \( X \) be a topological space and \( \{F_n\}_{n \in \mathbb{N}} \) be a sequence of functionals that \( \Gamma' \)-converges to \( F \). Let \( \{x_n\}_{n \in \mathbb{N}} \) be a sequence of quasi-minimizers. If \( x \) is a limit point of \( \{x_n\}_{n \in \mathbb{N}} \), then \( x \) is a minimizer of \( F \).

Based on the above statements, we are left to show that \( \{L_n\}_{n=1}^{\infty} \) is an equicoercive sequence of functionals that \( \Gamma' \)-converges to \( L \). We begin by proving the existence of the minimizers of \( L_n \) by referring the universal approximation theorem of the neural network.

**Theorem 3.5 (Theorem 2.1 in [1] (1996)).** Let \( K \) be a compact subset of \( \mathbb{R}^d \). Suppose there exists an open set \( \Omega \) containing \( K \) such that \( f \) lies in \( C^m(\Omega) \) for some \( m \in \mathbb{Z}_+^d \). If the activation function \( \sigma \) is in \( C^m(\mathbb{R}) \), then for any \( \epsilon > 0 \), there exists a neural network \( u_{nn}(x) = \sum_{i=1}^{h} c_i \sigma(w_i x + b_i) \) such that

\[
||D^\alpha(u_{nn}) - D^\alpha(f)||_{L^\infty(K)} < \epsilon, \forall \alpha \in \mathbb{Z}_+^d, |\alpha| \leq n.
\]

As a direct corollary of the theorem, the following proposition states that there always exists a neural network that makes the loss functional \( L_n \) sufficiently small.

**Proposition 3.6.** For given \( \epsilon > 0 \), there exists a neural network \( u_{nn} \) defined as in (3.5) such that \( L_n(u_{nn}) < \epsilon \), for the Helmholtz equation given in (16).
Remark 3.7. The same argument can easily be made for the viscous Burgers equation (19) and the Klein–Gordon equation (23).

We next show that the sequence of proposed loss functions \( \{L_n\}_{n \in \mathbb{N}} \) is an equicoercive sequence of functionals for three benchmark equations.

**Theorem 3.8.** The sequence \( \{L_n\}_{n \in \mathbb{N}} \) is equicoercive in weak topology for the Helmholtz (16), viscous Burgers (19), and Klein–Gordon equations (23).

We are now ready to prove the convergence of dominant quasi-minimizers of the proposed loss functionals \( \{L_n\}_{n \in \mathbb{N}} \). The following theorem states the convergence by proving the \( \Gamma^* \)-convergence of the proposed loss functionals \( \{L_n\}_{n \in \mathbb{N}} \) to \( L \).

**Theorem 3.9.** Consider a sequence of quasi-minimizers \( \{u_n\}_{n \in \mathbb{N}} \) with respect to \( \{L_n\}_{n \in \mathbb{N}} \). Then, \( u_n \to u \) in the weak topology, where \( u \) is the minimizer of functional \( L \) (i.e., \( u \) is the solution of equation (4)). This holds for the Helmholtz (16), viscous Burgers (19), and Klein–Gordon equations (23).

To prove the above theorem, we need the uniform boundedness of the sequence \( \{\|\lambda_n\|_{L^2(\partial \Omega)}\} \). The next lemma states that for a sufficiently large penalty parameter \( \beta \), we have the uniform boundedness of \( \{\|\lambda_n\|_{L^2(\partial \Omega)}\} \).

**Lemma 3.10.** Consider a sequence of quasi-minimizers \( \{u_n\}_{n \in \mathbb{N}} \) with respect to \( \{L_n\}_{n \in \mathbb{N}} \) for a sufficiently large \( \beta \). Then, the corresponding \( \|\lambda_n\|_{L^2(\partial \Omega)} \) is bounded for all \( n \in \mathbb{N} \).

Remark 3.11. In convex optimization literature, a large value of \( \beta \) stabilizes the augmented Lagrangian method. Since the uniform boundedness of \( \{\|\lambda_n\|_{L^2(\partial \Omega)}\} \) is essential to guarantee the \( \Gamma^* \)-convergence, a large \( \beta \) stabilizes the proposed AL-PINNs as in convex optimization. We will numerically confirm the uniform boundedness of \( \{\|\lambda_n\|_{L^2(\partial \Omega)}\} \) in Section 4.1.

### 4. Numerical Experiments

We detail our experimental settings and results that demonstrate the superior performance of the proposed AL-PINNs from two different perspectives. First, we compare the approximation error of the AL-PINNs with those of other constrained optimization strategies, such as the penalty and Lagrange multiplier methods. In this comparative analysis, we observe that both the penalty and multiplier terms are indispensable to obtaining an accurate approximation.

Next, we compare the approximation error of the proposed method with those of several adaptive loss balancing algorithms. In this experiment, we provide evidence that AL-PINNs approximates the solution accurately, whereas the existing adaptive loss balancing algorithms fail to reduce the boundary error sufficiently.

Throughout this section, we denote the number of points for the residual loss by \( N_r \), the number of points for the boundary conditions by \( N_b \), and the number of points for the initial conditions by \( N_i \). We employ the hyperbolic tangent function as an activation function, and the ADAM optimizer proposed in Kingma & Ba (2014) for training.

#### 4.1. AL-PINNs as a deep constrained optimization method for PINNs

**Experimental Setup.** In this subsection, we provide several experimental results that showcase the superior performance of AL-PINNs compared with those of the penalty and standard Lagrange multiplier methods (see Section 2 for algorithms). We measure the relative \( L^2 \) error of the neural network solution \( u_{nn} \), given by \( \|u - u_{nn}\|_{L^2}/\|u\|_{L^2} \), for each algorithm, using the Helmholtz equation as a benchmark PDE. The equation reads as:

\[
\Delta u + u = f(x, y), \quad \text{for} \ (x, y) \in \Omega,
\]

\[
u(x, y) = 0, \quad \text{for} \ (x, y) \in \partial \Omega,
\]

where \( \Omega = [-1, 1] \times [-1, 1] \). If we take

\[
f(x, y) = -\pi^2 \sin(\pi x) \sin(4\pi y)
\]

\[- (4\pi)^2 \sin(\pi x) \sin(4\pi y) + \sin(\pi x) \sin(4\pi y),
\]

then it can readily be shown that \( u(x, y) = \sin(\pi x) \sin(4\pi y) \) is an analytic solution. The loss functions are given as:

\[
L^{(P)}_{\beta_n} \approx \frac{1}{N_r} \sum_{i=1}^{N_r} (\Delta u_{nn}(x_i) + u(x_i) - f(x_i))^2
\]

\[+ \frac{\beta_n}{N_B} \sum_{j=1}^{N_B} u^2_{nn}(x_j),
\]

\[
L^{(L)}_{\lambda_n} \approx \frac{1}{N_r} \sum_{i=1}^{N_r} (\Delta u_{nn}(x_i) + u(x_i) - f(x_i))^2
\]

\[+ \frac{1}{N_B} \sum_{j=1}^{N_B} \lambda_n(x_j) u_{nn}(x_j),
\]

\[
L^{(A)}_{\lambda_n, \beta} \approx \frac{1}{N_r} \sum_{i=1}^{N_r} (\Delta u_{nn}(x_i) + u(x_i) - f(x_i))^2
\]

\[+ \frac{\beta}{N_B} \sum_{j=1}^{N_B} u^2_{nn}(x_j) + \frac{1}{N_B} \sum_{j=1}^{N_B} \lambda_n(x_j) u_{nn}(x_j),
\]

where \( L^{(P)}_{\beta_n} \) denotes a loss function for the penalty method, \( L^{(L)}_{\lambda_n} \) denotes the Lagrange multiplier method, \( L^{(A)}_{\lambda_n, \beta} \) denotes AL-PINNs, \( \beta_n \to \infty \), and \( \beta \) is a predefined constant.
this subsection, the layers of the neural networks consist of neurons 2-256-256-1.

**Results.** Figure 1 shows the trajectories of the total loss given in (3) and the relative $L^2$ error while training with the penalty method with a linearly increasing sequence of $\{\beta_n\}_{n=1}^{50000}$, the Lagrange multiplier method, and our AL-PINNs with $\beta = 1$. We observe that a neural network hardly learns the solution of the Helmholtz equation when training with the Lagrange multiplier method. This finding coincides with the theoretical observation made in Remark 3.11 that there exists a lower bound for $\beta$ to achieve the boundedness of the sequence $\{\lambda_n\}$. We also observe that both the total loss and the relative error rapidly converge to relatively high values as $\beta_n$ increases. This phenomenon is somewhat explained by the fact that a large value of $\beta$ causes the dominance of the boundary condition over the residual loss, which makes the training unstable. Finally, we can see that our AL-PINNs results in a much smaller relative error (about 40 times) than the penalty method.

**Figure 1.** Left: Trajectories of the total loss given in (3) for the penalty method (green), Lagrange multiplier method (orange), and the proposed AL-PINNs (blue). Right: Trajectories of the relative $L^2$ for the same algorithms. Here, we set $\beta_n = \beta$ for the penalty method, $\eta_\lambda = 10^{-4}$ for the Lagrange multiplier method, and $\eta_\lambda = 10^{-4}, \beta = 1$ for the proposed AL-PINNs.

Figure 2 shows the analytic solution and pointwise absolute errors for the training algorithms. Due to the training instability of the penalty method, we set $\beta_n \equiv \beta$ as in the original work by Raissi et al. (2019). We observe that most errors arise from the near boundary points in both the penalty and Lagrange multiplier methods. This indicates that the boundary condition is indeed a critical factor for a relatively high error level. As it exhibits negligible boundary errors, we can conclude that the proposed loss function given in (5) is the best relaxation method of the boundary condition into the loss function.

**Figure 2.** Top left: True solution of the Helmholtz equation. Top right: Pointwise absolute error for the penalty method with $\beta_n \equiv 1$. Bottom left: Pointwise absolute error for the Lagrange multiplier method with $\eta_\lambda = 10^{-4}$. Bottom right: Pointwise absolute error for the proposed AL-PINNs with $\eta_\lambda = 10^{-4}, \beta = 1$. Errors are computed using the best model over 50,000 training epochs.

$\beta$ plays a significant role in training a neural network with both the penalty method and our AL-PINNs. In Figure 3, we provide the relative $L^2$ errors for the penalty method with a constant penalty parameter and our AL-PINNs for different values of $\beta$. The left panel of Figure 3 shows the relative errors for different values of $\beta$ after 50,000 training epochs. One can see that the relative errors highly depend on the values of $\beta$ in both cases, yet the proposed AL-PINNs uniformly outperforms (up to 70 times) the penalty method. The right panel of Figure 3 supports the uniform boundedness argument of $\|\lambda_n\|_{L^2(\partial\Omega)}$ stated in Lemma 3.10 throughout the training. As we can see in Figure 3, the $L^2$ norm of $\lambda_n$ converges to a certain value for all $\beta$ in $\{1, 10, 100, 1000\}$ even with a relatively high value of $\eta_\lambda = 1$. Thus, we can say that the sequence $\{\lambda_n\}$ has an upper bound, and an important condition to guarantee the convergence is satisfied.

**Figure 3.** Left: Relative $L^2$ errors for the penalty method with constant $\beta_n \equiv \beta$ and the proposed AL-PINNs with the same $\beta$. Right: The $L^2$ norm of $\lambda_n$ in training epoch for different $\beta$'s.
### Table 1. Average relative $L^2$ errors and standard deviations over 10 different trials for the Helmholtz equation.

| Algorithm | PINNs | SA | LRA | NTK | AL-PINNs |
|-----------|------|----|-----|-----|---------|
| M1        | 5.12e-01 ± 2.08e-01 | 2.32e-01 ± 5.13e-02 | 2.85e-01 ± 8.50e-02 | 3.80e-01 ± 1.09e-01 | 6.44e-03 ± 3.65e-03 |
| M2        | 2.11e-02 ± 4.82e-03 | 2.40e-02 ± 2.26e-03 | 1.06e-02 ± 1.91e-03 | 2.18e-02 ± 6.05e-03 | 6.00e-04 ± 1.13e-04 |
| M3        | 1.14e-01 ± 3.28e-02 | 9.65e-02 ± 2.27e-02 | 3.61e-02 ± 9.64e-03 | 1.23e-01 ± 1.88e-02 | 4.90e-04 ± 6.47e-05 |
| M4        | 1.93e-02 ± 4.78e-03 | 2.43e-02 ± 3.18e-03 | 8.89e-03 ± 1.05e-03 | 2.25e-02 ± 4.16e-03 | 7.46e-04 ± 1.10e-04 |

### 4.2. AL-PINNs as an adaptive Loss Balancing Algorithm for PINNs

**Baselines.** One can readily see that the proposed method naturally belongs to a class of adaptive loss balancing algorithms. In this subsection, we demonstrate the superior performance of the proposed AL-PINNs compared with the vanilla Physics-Informed Neural Networks (PINNs), a Soft Attention mechanism (SA) proposed in McClenny & Braga-Neto (2020), a Learning Rate Annealing algorithm (LRA) presented in Wang et al. (2021), and a loss balancing algorithm via the eigenvalues of the Neural Tangent Kernel (NTK) proposed in Wang et al. (2022). We use the Helmholtz, viscous Burgers, and the Klein–Gordon equations as benchmark PDEs, as they are widely used for this purpose in PINNs literature (For example, see Son et al. (2021), McClenny & Braga-Neto (2020), Wang et al. (2021), Bischof & Kraus (2021)). Although Wang et al. (2022) did not investigate those equations, the idea is easily generalizable to those equations. We compare the relative $L^2$ error of the proposed AL-PINNs with those of the vanilla PINNs, SA, LRA, and NTK algorithms using the above PDEs. We provide detailed equations and loss functions in Appendix A.

**Experimental Setup.** We compare the algorithms for four different neural network architectures, namely M1, M2, M3, and M4 in Tables 1, 2. M1 consists of 8 hidden layers with 64 neurons, M2 consists of 2 hidden layers with 256 neurons, M3 denotes M1 equipped with residual connections, and M4 denotes M2 equipped with residual connections. We uniformly sampled the test dataset from the domain of each PDE and computed the relative $L^2$ error of the neural network solution $u_{nn}$, given by $\|u - u_{nn}\|_{L^2}/\|u\|_{L^2}$, on the test dataset. For each training algorithm-architecture pair, we train 10 instances of neural networks with the Kaiming uniform initialization method presented in He et al. (2015). We report the average relative $L^2$ errors and the standard deviations across 10 trials. The hyperparameter configurations for $\beta, \eta_\alpha, \eta_\lambda$ are provided in appendix B.

**Helmholtz equation.** We define the loss function $L^{(A)}_{\lambda, \eta, \beta}$ as in (11), by using the proposed AL-PINNs. We train a neural network on a fixed uniform rectangular grid where $N_r = 2500$ and $N_B = 200$. We train the neural networks for 10000 epochs, and use the early stopping strategy as the stopping criteria. We summarized the average test errors and standard deviations for the Helmholtz equation in Table 1.

![Figure 4. Pointwise absolute errors of the baseline algorithms for the Helmholtz equation. All adaptive loss balancing algorithms suffer from boundary errors except our AL-PINNs.](image)

Figure 4 shows the analytic solution of the Helmholtz equation and pointwise absolute errors for the baseline algorithms with the model M2. All adaptive loss balancing algorithms result in severe boundary errors except for our AL-PINNs. This implies that existing adaptive loss balancing algorithms fail to find optimal $\lambda$’s to achieve an accurate approximation. On the other hand, the proposed AL-PINNs converges to a highly accurate approximate solution with a uniform error distribution. Table 1 shows that the proposed AL-PINNs achieves a much smaller relative error than other adaptive loss balancing algorithms throughout the models M1-M4.

**Viscous Burgers equation.** The viscous Burgers’ equation (12) admits an analytic solution presented in Basdevant et al. (1986), which we use to compute the relative $L^2$ error. We define the loss function $L^{(A)}_{\lambda, \eta, \beta}$ as in (13) by using the proposed AL-PINNs. We train the neural networks on a fixed uniform rectangular grid with $N_r = 2500$, $N_B = 100$, and $N_I = 50$, for 10000 epochs, and employ the early stopping strategy as the stopping criteria.
Table 2. Average relative $L^2$ errors and standard deviations over 10 different trials for the Burgers equation.

|                  | PINNs         | SA            | LRA           | NTK           | AL-PINNs       |
|------------------|---------------|---------------|---------------|---------------|----------------|
| Burgers' equation| 8.92e-02 ± 2.43e-02 | 9.80e-02 ± 5.54e-02 | 1.48e-01 ± 4.56e-02 | 1.22e-01 ± 3.58e-02 | 5.45e-02 ± 9.41e-03 |
| M2               | 7.29e-02 ± 7.14e-03 | 8.40e-02 ± 8.48e-03 | 6.64e-02 ± 5.86e-03 | 6.61e-02 ± 8.13e-03 | 5.91e-02 ± 6.37e-03 |
| M3               | 4.85e-02 ± 5.95e-03 | 4.71e-02 ± 1.82e-02 | 4.38e-02 ± 6.39e-03 | 4.52e-02 ± 6.50e-03 | 4.10e-02 ± 7.32e-03 |
| M4               | 1.21e-01 ± 3.26e-02 | 1.06e-01 ± 2.16e-02 | 6.34e-02 ± 6.39e-03 | 7.40e-02 ± 1.21e-02 | 5.89e-02 ± 4.22e-03 |

Table 3. Average relative $L^2$ errors and standard deviations over 10 different trials for the Klein–Gordon equation.

|                  | PINNs         | SA            | LRA           | NTK           | AL-PINNs       |
|------------------|---------------|---------------|---------------|---------------|----------------|
| Klein–Gordon equation | 3.86e-01 ± 1.21e-01 | 2.45e-01 ± 1.23e-01 | 2.39e-01 ± 4.62e-02 | 8.11e-01 ± 2.77e-01 | 1.42e-02 ± 7.34e-03 |
| M2               | 5.25e-02 ± 1.42e-02 | 4.32e-02 ± 1.21e-02 | 2.22e-02 ± 1.30e-02 | 1.33e-02 ± 6.80e-03 | 5.73e-03 ± 1.45e-03 |
| M3               | 1.10e-01 ± 4.93e-02 | 1.40e-01 ± 4.77e-02 | 7.19e-02 ± 2.56e-02 | 3.01e-02 ± 1.17e-02 | 7.35e-03 ± 1.98e-03 |
| M4               | 5.74e-02 ± 1.76e-02 | 3.65e-02 ± 1.09e-02 | 2.35e-02 ± 1.26e-02 | 1.24e-02 ± 3.88e-03 | 5.28e-03 ± 1.37e-03 |

Figure 5 shows the analytic solution and pointwise absolute errors for the vanilla PINNs, an adaptive loss balancing algorithm using a soft attention mechanism (SA), and the proposed AL-PINNs with the model M1. McClellan & Braga-Neto [2020] argued that PINNs suffers from an accuracy problem where the solution has a sharp spatio-temporal transition. For example, the solution of the viscous Burgers equation (12) exhibits a sharp transition near $x = 0$ (the horizontal line). The absolute errors in Figure 5 show that the proposed AL-PINNs results in a much smaller error near $x = 0$, compared to those of other methods. This result demonstrates that the proposed AL-PINNs outperforms both the vanilla PINNs and the soft attention mechanism in a problem with sharp spatio-temporal transitions. We summarized the average relative $L^2$ errors and standard deviations in Table 2.

Klein–Gordon equation. The equation and proposed loss function are given in (14) and (15), respectively. We train a neural network on a fixed uniform mesh with $N_r = 2500$, $N_B = 100$, and $N_I = 50$. We train the neural networks for 10,000 epochs and employ the early stopping strategy as the stopping criteria. We summarize the results in Table 3 which shows that the proposed AL-PINNs outperforms other loss balancing algorithms for all network architectures we considered.

5. Conclusions

In this paper, we proposed AL-PINNs, a convergence-guaranteed highly accurate adaptive loss balancing algorithm for PINNs. We proved the convergence of sequence generated by the proposed method in Section 3. We evaluated the proposed method in two different aspects. In Section 4.1 we observed that the penalty and multiplier terms should both be considered in the loss function to obtain an accurate approximation. In Section 4.2, we demonstrated the superior performance of AL-PINNs compared with that of other loss balancing algorithms in various settings. To summarize, we believe that our AL-PINNs is a universal framework that can be successfully applied to a variety of PDEs.
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A. PDEs and Loss Functions

Helmholtz equation
The 2-D Helmholtz equation reads:

\[
\begin{align*}
\Delta u + u &= f(x, y), \quad \text{for } (x, y) \in \Omega, \\
u(x, y) &= 0, \quad \text{for } (x, y) \in \partial \Omega,
\end{align*}
\]

where \( \Omega = [-1, 1] \times [-1, 1] \). If we take

\[
f(x, y) = -\pi^2 \sin(\pi x) \sin(4\pi y) - (4\pi)^2 \sin(\pi x) \sin(4\pi y) + \sin(\pi x) \sin(4\pi y),
\]

then one can readily show that \( u(x, y) = \sin(\pi x) \sin(4\pi y) \) is an analytic solution. The proposed loss function reads as:

\[
L_{\lambda, \beta}^{(\text{H})} \approx \frac{1}{N_t} \sum_{i=1}^{N_t} (\Delta u_{nn}(x_i) + u(x_i) - f(x_i))^2 + \frac{\beta}{N_B} \sum_{j=1}^{N_B} u_{nn}^2(x_j) + \frac{1}{N_B} \sum_{j=1}^{N_B} \lambda_n(x_j) u_{nn}(x_j),
\]

Viscous Burgers equation
We consider the viscous Burgers equation:

\[
\begin{align*}
\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( \frac{1}{2} u^2 - cu \right) &= 0, \quad \text{for } (t, x) \in [0, 1] \times [-1, 1], \\
u(0, x) &= -\sin(\pi x), \quad \text{for } x \in [-1, 1], \\
u(t, -1) &= u(t, 1) = 0, \quad \text{for } t \in [0, 1],
\end{align*}
\]

for \((t, x) \in [0, 1] \times [-1, 1]\), and \( c = \frac{0.01}{\pi} \). This setting is the same as in McClenny & Braga-Neto [2020], Kim et al. [2021]. The viscous Burgers’ equation admits an analytic solution presented in Basdevant et al. [1986]. In this case, the proposed loss function reads as:

\[
L_{\lambda, \beta}(\theta) \approx \frac{1}{N_t} \sum_{i=1}^{N_t} \left( \frac{\partial t}{\partial t} u_{nn}(t_i, x_i) + \frac{\partial}{\partial x} \left( \frac{1}{2} u_{nn}^2 - c\partial x u_{nn} \right)(t_i, x_i) \right)^2 \\
+ \frac{\beta}{N_B} \sum_{j=1}^{N_B} (u_{nn}(0, x_j) + \sin(\pi x_j))^2 + \frac{1}{N_B} \sum_{j=1}^{N_B} (\lambda_n^{(1)}(x_j))(u_{nn}(0, x_j) + \sin(\pi x_j)) \\
+ \frac{\beta}{N_B} \sum_{k=1}^{N_B} (u_{nn}(t_k, -1) - u_{nn}(t_k, 1))^2 + \frac{1}{N_B} \sum_{k=1}^{N_B} (\lambda_n^{(2)}(t_k))(u_{nn}(t_k, -1) - u_{nn}(t_k, 1)).
\]

Klein–Gordon equation
The Klein–Gordon equation we consider reads:

\[
\begin{align*}
\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + uu &= f(t, x), \quad \text{for } (t, x) \in [0, 1] \times [0, 1], \\
u(0, x) &= g_1(x), \quad \text{for } x \in [0, 1], \\
\frac{\partial u}{\partial t}(0, x) &= g_2(x), \quad \text{for } x \in [0, 1], \\
u(t, x) &= h(t, x), \quad \text{for } (t, x) \in [0, 1] \times \{0, 1\},
\end{align*}
\]

where \( f, g_1, g_2, h \) are computed using a fabricated solution

\[
u(t, x) = x \cos(5\pi t) + (tx)^3;
\]
as in [Wang et al., 2021]. In this example, the proposed loss function reads as:

\[
\mathcal{L}_{\lambda_n, \beta}(\theta) \approx \frac{1}{N_r} \sum_{i=1}^{N_r} \left( \partial_t^2 u_{nn}(x_i) - \partial_x^2 u_{nn}(x_i) + u_{nn}^3(x_i) - f(x_i) \right)^2 \\
+ \frac{\beta}{N_t} \sum_{j=1}^{N_t} (u_{nn}(0, x_j) - g_1(x_j))^2 + \frac{1}{N_t} \sum_{j=1}^{N_t} (\lambda_{1}(x_j))(u_{nn}(0, x_j) - g_1(x_j)) \\
+ \frac{\beta}{N_t} \sum_{j=1}^{N_t} (\partial_t^2 u_{nn}(0, x_j) - g_2(x_j))^2 + \frac{1}{N_t} \sum_{j=1}^{N_t} (\lambda_{2}(x_j))(\partial_t^2 u_{nn}(0, x_j) - g_2(x_j)) \\
+ \frac{\beta}{N_B} \sum_{k=1}^{N_B} (u_{nn}(t_k, x_k) - h(t_k, x_k))^2 + \frac{\beta}{N_B} \sum_{k=1}^{N_B} (\lambda_{3}(t_k, x_k))(u_{nn}(t_k, x_k) - h(t_k, x_k)).
\]

(15)

B. Hyperparameters

For all algorithm-architecture pairs in the tables in Section 4, we test the learning rate \( \eta \) from \{10^{-3}, 10^{-4}, 10^{-5}\}. We choose \( \beta \) from \{10^{0}, 10^{1}, 5 \times 10^{2}, 10^{2}, 5 \times 10^{2}, 10^{3}, 10^{4}\} and \( \eta_\theta \) from \{10^{0}, 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}\} and report the best error. We set the initial value of the multiplier to be \( \lambda_0 = \{0, 0, \ldots, 0\} \) for the proposed AL-PINNs. Table 4 shows the best hyperparameters for each equation.

**Table 4.** Best hyperparameter configurations.

| Best Hyperparameters | Helmholtz equation | Viscous Burgers equation | Klein–Gordon equation |
|----------------------|-------------------|--------------------------|-----------------------|
| \( \beta \)         | \( \eta_\lambda \) | \( \eta_\theta \)        | \( \beta \)          | \( \eta_\lambda \) | \( \eta_\theta \) | \( \beta \) | \( \eta_\lambda \) | \( \eta_\theta \) |
| M1                   | \( 10^3 \)        | 1                        | \( 10^{-3} \)         | \( 1 \)             | \( 10^{-4} \)     | \( 5 \times 10^2 \) | 1         | \( 10^{-3} \)         |
| M2                   | \( 5 \times 10^2 \) | 1                        | \( 10^{-4} \)         | \( 1 \)             | \( 10^{-3} \)     | \( 5 \times 10^2 \) | 1         | \( 10^{-3} \)         |
| M3                   | \( 10^3 \)        | 1                        | \( 10^{-4} \)         | \( 1 \)             | \( 10^{-3} \)     | \( 5 \times 10^2 \) | 1         | \( 10^{-3} \)         |
| M4                   | \( 5 \times 10^2 \) | 1                        | \( 10^{-3} \)         | \( 1 \)             | \( 10^{-3} \)     | \( 5 \times 10^2 \) | 1         | \( 10^{-3} \)         |

For the baseline algorithms, we followed the best hyperparameter settings provided in each paper. For example, we set the initial \( \lambda \) to be \( (1, 1, \ldots, 1) \) for SA method in [McCleny & Braga-Neto, 2020]. For the LRA method, we set \( \alpha = 0.1 \) and the initial \( \lambda \) to be ones, as in [Wang et al., 2021].

C. Proof of Theorems

**Theorem 3.3.** Let \( X \) be a reflexive Banach space and \( \{F_n\}_{n \in \mathbb{N}} \) be a sequence of equicoercive functionals on \( X \) that \( \Gamma' \)-converges to \( F \) with a unique minimizer \( x \). Then, every sequence \( \{x_n\}_{n \in \mathbb{N}} \) of quasi-minimizers of \( \{F_n\}_{n \in \mathbb{N}} \) converges weakly to \( x \).

**Proof.** If \( r > \inf F \), then \( x_k \) is contained in the bounded set \( \bigcup_{n \in \mathbb{N}} \{x \in X : F_n(x) \leq r\} \) for a sufficiently large \( k \) by the inequality

\[
\inf_{x \in X} F \geq \lim_{n \to \infty} \sup_{x \in X} F_n = \lim_{n \to \infty} \sup_{x \in X} (F_n + \delta_n).
\]

The reflexivity of \( X \) ensures that \( \{x_n\}_{n \in \mathbb{N}} \) has a weakly convergent subsequence \( \{x_{nk}\}_{k \in \mathbb{N}} \), and the limit point \( x \) should be a unique minimizer of \( F \) by Lemma 3.4. Suppose that there exists a subsequence \( \{x_{nm}\}_{m \in \mathbb{N}} \) and an element \( G \) in \( X^* \) such that \( \{G(x_{nm})\}_{m \in \mathbb{N}} \) not converging to \( G(x) \). \( x_{nm} \) attains a further subsequence which converges to \( x \) by the reflexivity of \( F \) so that a contradiction arises. Therefore, \( x_n \) converges to \( x \) weakly. Along with the Admissible limit point property, we conclude that \( x \) lies in \( F_A \) so that \( F \) indeed attains its minimum at \( x \).

\[\Box\]
Lemma 3.4. Let $X$ be a topological space and $\{F_n\}_{n \in \mathbb{N}}$ be a sequence of functionals that $\Gamma'$-coverves to $F$. Let $\{x_n\}_{n \in \mathbb{N}}$ be a sequence of quasi-minimizers. If $x$ is a limit point of $\{x_n\}_{n \in \mathbb{N}}$, then $x$ is a minimizer of $F$.

Proof. First, we consider a recovery sequence $\{y_n\}_{n \in \mathbb{N}}$ for $y \in F_A$ to establish the following inequalities.

$$F(y) = \lim_{n \to \infty} F_n(y_n) = \limsup_{n \to \infty} F_n(y_n) \geq \liminf_{n \to \infty} F_n(y_n).$$

Taking the infimum over $y$, we reformulate the inequality to $\inf_x F \geq \limsup_{n \to \infty} (\inf_x F_n)$. By the admissible limit point property, $x \in F_A$ and therefore, the liminf inequality yields the following.

$$F(x) \leq \liminf_{n \to \infty} F_n(y_n) \leq \limsup_{n \to \infty} (\inf_x F_n) \leq \limsup_{n \to \infty} (\inf_x F_n) \leq \inf_X(F).$$

Consequently, $x$ should be a minimizer of $F$. \qed

Proposition 3.6. For given $\epsilon > 0$, there exists a neural network $u_{nn}$ defined as in 3.5 such that $L_n(u_{nn}) < \epsilon$, for the Helmholtz equation given in [16].

Proof. Let $\epsilon > 0$ be given and let $u$ denotes a strong solution of the Helmholtz equation [16]. By theorem 3.5, there exists $u_{nn}(x, y)$ defined as in theorem 3.5 such that

$$\max_{|\alpha| \leq 2} \|D^\alpha(u) - D^\alpha(u_{nn}(x, y))\|_{L^\infty(\Omega)} < \epsilon.$$

Then,

$$L_n(u_{nn}) = \|\Delta u_{nn}(x, y) + k^2 u_{nn}(x, y) - q(x, y)\|_{L^2(\Omega)} + \|u_{nn}(x) - g(x)\|_{L^2(\partial \Omega)}$$

$$= \|\Delta (u_{nn}(x, y) - u(x, y)) + k^2 (u_{nn}(x, y) - u(x, y))\|_{L^2(\Omega)} + \|u_{nn}(x, y) - u(x, y)\|_{L^2(\partial \Omega)}$$

$$\leq \|\Delta (u_{nn}(x, y) - u(x, y))\|_{L^2(\Omega)} + \|k^2 (u_{nn}(x, y) - u(x, y))\|_{L^2(\Omega)} + \|u_{nn}(x, y) - u(x, y)\|_{L^2(\partial \Omega)}$$

$$\leq C\epsilon$$

for some $C > 0$. This completes the proof. \qed

Theorem 3.8. The sequence $\{L_n\}_{n \in \mathbb{N}}$ is equicoercive in weak topology for the Helmholtz [16], viscous Burgers [19], and Klein–Gordon equations [23].

Proof of Theorem 3.8 for the Helmholtz equation

The Helmholtz equation reads:

$$N(u) := \Delta u(x, y) + k^2 u(x, y) = f(x, y), \quad (x, y) \in \Omega$$

$$u = g, \quad (x, y) \in \partial \Omega$$

(16)

for a constant $k$. In this paper, we only consider the case that $\Omega$ is a rectangle $[a, b] \times [c, d]$ and there exists $h \in H^2(\Omega)$ such that $T(h) = g$ for the trace operator $T$. There are existence and uniqueness theorems for linear elliptic equation. Let us denote the set of all eigenvalues of Laplace operator $L(u) := -\Delta u$ by $\Sigma$ (i.e. if $k^2 \notin \Sigma$, then $L(u) := -\Delta u - k^2 u = f$ has a unique solution with $u = 0$ on $\partial \Omega$). Then, the set $\Sigma$ is at most countable (see theorem 5 in Section 6.2 of Evans [1998]) and the following theorem holds.

Theorem C.1 (Thm 6 in Sec 6.2 of Evans [1998]). Let $f \in L^2(\Omega)$. Suppose $k^2 \notin \Sigma$ and let $u \in H^1_0(\Omega)$ be the unique solution of the following equation.

$$\Delta u + k^2 u = f, \quad in \quad \Omega,$$

$$u = 0, \quad on \quad \partial \Omega.$$  

(17)

Then, there exist a constant $C$ which depends on $k^2$ and $\Omega$ such that the following inequality holds.

$$\|u\|_{L^2(\Omega)} \leq C(\|f\|_{L^2(\Omega)}).$$
Note that the constant $C$ does not depend on $f$. Since $f$ is a component of the loss function, the above theorem implies the boundedness of $\|u\|_{L^2(\Omega)}$ under the exact boundary condition. Now we refer the theorem about higher regularity of the solution. That is, the solution of (17) indeed lies in $H^2(\Omega)$.

**Theorem C.2** (Thm 4.3.1.4 in Grisvard [2011]). Suppose that $\Omega$ is bounded open and its boundary $\partial \Omega$ is the union of finite line segments. Then, we can have the following estimate of $\|u\|_{H^2(\Omega)}$ when $u \in H^1(\Omega)$ is the solution of (17).

$$\|u\|_{H^2(\Omega)} \leq C(\|f\|_{L^2(\Omega)} + \|u\|_{L^2(\Omega)}),$$

where $C$ is a constant depending on $k^2$ and $\Omega$.

Suppose that the neural network $w$ satisfies the following.

$$\begin{align*}
\Delta w + k^2 w &= f^* , & \text{in } & \Omega, \\
w &= g^* , & \text{on } & \partial \Omega.
\end{align*}$$

Under the whole training process, we assume that the uniform boundedness of $\|\frac{d}{dy}(g^*(a, y))\|_{L^2((a, c) \times [b, d])}$ and $\|\frac{d}{d^2 y}(g^*(x, b))\|_{L^2([a, c] \times \{b\})}$, $\|\frac{d}{d^2 y}, g^*(x, d))\|_{L^2([a, c] \times \{d\})}$ for $x \in (a, c)$. That is, there exists a constant $\epsilon > 0$ such that

$$\|\frac{d}{d^2 y}(g^*(a, y))\|_{L^2((a, c) \times [b, d])} + \|\frac{d}{d^2 y}, g^*(x, c))\|_{L^2([a, c] \times \{c\})} + \|\frac{d}{d^2 y}, g^*(x, b))\|_{L^2([a, c] \times \{b\})} + \|\frac{d}{d^2 y}, g^*(x, d))\|_{L^2([a, c] \times \{d\})} \leq \epsilon$$

Note that the assumption implies the fact that $\|g^*(a, y)\|_{L^\infty([a, c] \times \{b\})}$ is uniformly bounded during the training process. To explain it more precisely, Morrey’s inequality yields that

$$\begin{align*}
\|g^*(a, y)\|_{L^\infty([a, c] \times \{b\})} &\leq C\|g^*(a, y)\|_{H^1([a, c] \times \{b\})}, \\
\|d/dy (g^*(a, y))\|_{L^\infty([a, c] \times \{b\})} &\leq C\|d/dy (g^*(a, y))\|_{H^1([a, c] \times \{b\})}.
\end{align*}$$

with the fact that $g^*(a, y)$ should be a smooth function since it is consistent with the smooth neural network $w$ on boundary. Therefore, the desired property of $\|g^*(a, y)\|_{L^2([a, c] \times \{b\})}$ is valid by the uniform boundedness of $\|g^*(a, y)\|_{L^2([a, c] \times \{b\})}$ which will be proved below. Now we are ready to prove the main theorem [C.3] for the Helmholtz equation.

**Proof.** We consider the case $k^2 \notin \Sigma$ where $\Sigma$ denote the spectrum of the Laplace operator. By assumption, there exists a harmonic polynomial $h_1(x, y) = a_0(x^2 - y^2) + a_1 x y + a_2 x + a_3 y + a_4 \in H^2(\Omega)$ which satisfies $h = g^*$ on the four vertices $[a, c], [a, d], [b, c]$ and $[b, d]$. And $h_2(x, y)$ defined as below lies in $H^2(\Omega)$ with uniformly bounded norm during the entire training process.

$$h_2(x, y) = \frac{x - c}{a - c} \cdot (g - h_1)(a, y) + \frac{x - a}{c - a} \cdot (g - h_1)(c, y) + \frac{y - d}{b - d} \cdot (g - h_1)(x, b) + \frac{y - b}{d - b} \cdot (g - h_1)(x, d) \in H^2(\Omega).$$

Now we estimate the difference $e := w - h = w - (h_1 + h_2)$. First of all, $e$ should satisfy the following equation.

$$\begin{align*}
\Delta e + k^2 e = f^* - \Delta h - k^2 h , & \text{ in } & \Omega, \\
e = 0 , & \text{on } & \partial \Omega.
\end{align*}$$

Using Theorem [C.1], we get the estimate for $\|e\|_{L^2(\Omega)}$ where $C$ is a constant which depends only on $k^2$ and $\Omega$.

$$\|e\|_{L^2(\Omega)} \leq C\|f^* - \Delta h - k^2 h\|_{L^2(\Omega)} \leq C(\|f^*\|_{L^2(\Omega)} + (1 + k^2)\|h\|_{H^2(\Omega)})$$

Now we can conclude that $w \in H^2(\Omega)$ with theorem [C.2].

$$\begin{align*}
\|w\|_{H^2(\Omega)} &\leq \|e\|_{L^2(\Omega)} + \|h\|_{H^2(\Omega)} \\
&\leq C(k^2, \Omega)(\|e\|_{L^2(\Omega)} + \|f^* - \Delta h - k^2 h\|_{L^2(\Omega)}) + \|h\|_{H^2(\Omega)} \\
&\leq C(k^2, \Omega)(C + 1)\|f^*\|_{L^2(\Omega)} + ((1 + k^2)CC(k^2, \Omega) + (1 + k^2)C(k^2, \Omega) + 1)\|h\|_{H^2(\Omega)}
\end{align*}$$
where $C(k^2, \Omega)$ denotes the constant for theorem C.2. Now, suppose that $L_n(w) \leq r$ for some $r \in \mathbb{R}$ and $n \in \mathbb{N}$. That is,

$$L_n(w) = \| Nw - f \|_{L^2(\Omega)}^2 + \beta \| Tw - g \|_{L^2(\Omega)}^2 + (\lambda_n, Tw - g)_{L^2(\Omega)}$$

$$= \| f^* - f \|_{L^2(\Omega)} + \beta \| g^* - g \|_{L^2(\Omega)} + (\lambda_n, g^* - g)_{L^2(\Omega)} \leq r.$$

By lemma 3.10 which covers the uniform boundedness of $\| \lambda_n \|_{L^2(\Omega)}$ during the whole training process, the Hölders inequality $(\lambda_n, Tw - g)_{L^2(\Omega)} \geq \| \lambda_n \|_{L^2(\Omega)} \| Tw - g \|_{L^2(\Omega)}$ implies the fact that $\| g^* - g \|_{L^2(\Omega)}$ is bounded by constant depending on $r$. To explain in more precisely, note that $\lambda_n$ is an interval $[a, b]$ and $T$ is a fixed constant. Without loss of generality, set $a = 0$ and $b = 1$. Here, we note the solution space which is necessary to deal with the existence and uniqueness of the solution. The definition of anisotropic Sobolev space $H^{1,2}(R)$ is as follows.

$$H^{1,2}(R) = \{ u \in L^2(R) | \partial_t u \in L^2(R), \partial_x u \in L^2(R), \partial_x^2 u \in L^2(R) \},$$

where $R = \Omega \times [0, T]$ and $\| u \|_{L^2(R)} = \| u \|_{L^2([0, T]; L^2(\Omega))}$ denotes $(\int_0^T \| u(t, \cdot) \|_{L^2(\Omega)}^2 dt)^{1/2}$. The existence and uniqueness theorem for equation (19) are as follows.

**Theorem C.3. (Thm 1.2 in Benia & Sadallah 2016)** For the initial condition $w_0(x)$ which is contained in $H^1_0(\Omega)$, the unique weak solution of equation (19) exists in $H^{1,2}(R)$.

We would like to introduce an assumption before we discuss the equi-coercivity. Let $w$ denotes the smooth approximation of the solution $u$ such that

$$\partial_t w + \frac{1}{2} \partial_x^2 w^2 - \nu \partial_x^2 w = f, \quad (t, x) \in [0, T] \times \Omega,$$

$$w(0, x) = g(x), \quad x \in \Omega,$$

$$w(t, a) = h_1(t), w(t, b) = h_2(t), \quad t \in [0, T].$$

We assume the uniform boundedness of $\| \partial_t h_1(t) \|_{L^2([0, T])}$ and $\| \partial_t h_2(t) \|_{L^2([0, T])}$ for the entire training process. That is, there exists a constant $\epsilon > 0$ such that the boundary functions $g(x)$, $h_1(t)$ and $h_2(t)$ satisfy the following.

$$\| \frac{d}{dx} g(x) \|_{L^2([0, T])}, \| \frac{d}{dt} h_1(t) \|_{L^2([0, T])}, \| \frac{d}{dt} h_2(t) \|_{L^2([0, T])} \leq \epsilon.$$
where $f^* = f - \partial_t I - I \partial_x I - \nu \partial_x^2 I$ and $g^* = g(x) - g(0)(1 - x) - g(1)x$. On the one hand, Morrey’s inequality gives the inequality $g(0) = h_1(0) \leq \|h_1(t)\|_{L^\infty(0,T)} \leq C_1\|h_1(t)\|_{H^1(0,T)}$ so that $g^* \in H^1(\Omega)$ when $h_1(t) \in L^2([0,T])$. By multiplying $e$ to the first equation and integrating over $\Omega$ with integration by parts, we derive the following equation.

$$
\frac{1}{2} \frac{d}{dt} \|e(t, \cdot)\|_{L^2(\Omega)}^2 + \nu \|e_x(t, \cdot)\|_{L^2(\Omega)}^2 = \int_\Omega f^* e dx + \nu \int_{\partial \Omega} e \partial_x e \cdot ndS - \int_\Omega e^2 \partial_x e dx - \int_\Omega e^2 \partial_x I dx - \int_\Omega I e \partial_x e dx
$$

By Hölder’s inequality and scaled version of Cauchy’s inequality with small $\eta > 0$, we have

$$
\int_\Omega f^* e dx \leq \int_\Omega \left( \frac{f^*}{2} \right) + \frac{\nu}{2} \frac{d}{dt} \|e(t, \cdot)\|_{L^2(\Omega)}^2 + \frac{1}{2} \|e(t, \cdot)\|_{L^2(\Omega)}^2 + \|e(t, \cdot)\|_{L^2(\Omega)}^2 \|\partial_x I\|_{L^2(\Omega)}^2
$$

$$
\int_{\partial \Omega} e \partial_x e \cdot ndS = e(t,1) \partial_x e(t,1) - e(t,0) \partial_x e(t,0) = 0
$$

$$
\int_\Omega e^2 \partial_x e dx = \int_\Omega \frac{1}{3} \nu \cdot ndS = 0
$$

$$
\int_\Omega e^2 \partial_x I dx \leq \int_\Omega \left( \frac{e^2}{2} + \frac{\nu^2}{2} \right) \frac{d}{dt} \|\partial_x I\|_{L^2(\Omega)}^2 + \|\partial_x I\|_{L^2(\Omega)}^2 \|e\|_{L^2(\Omega)}^2
$$

$$
\int_\Omega I e \partial_x e dx \leq \int_\Omega \frac{I}{4\eta} \|e\|_{L^2(\Omega)}^2 \|\partial_x e\|_{L^2(\Omega)}^2 + \eta \|\partial_x e\|_{L^2(\Omega)}^2
$$

Since $\eta > 0$ is arbitrary small, we may assume that $2\eta < \nu$. Combining all estimates, we have the following upper bound of $d/dt(\|u\|_{L^2(\Omega)})$.

$$
\frac{d}{dt} \|e\|_{L^2(\Omega)}^2 + \nu \|\partial_x e\|_{L^2(\Omega)}^2 \leq (2 + \|\partial_x I\|_{L^2(\Omega)}^2 + \frac{1}{2\eta} \|\partial_x I\|_{L^2(\Omega)}^2) \|e\|_{L^2(\Omega)}^2 + \|f^*\|_{L^2(\Omega)}^2
$$

Then, by the Grönwall inequality,

$$
\|e\|_{L^2([0,T] \times \Omega)} \leq T \sup_{0 \leq t \leq T} \|e\|_{L^2(\Omega)}^2
$$

$$
\leq T \exp\left( 2T + \|\partial_x I\|_{L^2(\Omega)}^2 + \frac{1}{2\eta} \|\partial_x I\|_{L^2(\Omega)}^2 \right) \left( \|g^*\|_{L^2(\Omega)}^2 + \|f^*\|_{L^2(\Omega)}^2 \right)
$$

for some constant $C$ depending only on $r, T$. Now we consider the case that the neural network $w$ whose image by $L_n(w)$ are bounded for some $n \in \mathbb{N}$. Suppose that

$$
L_n(w) = L(w) + \langle \lambda_1(x), w(0, x) - u_0(x) \rangle_{L^2(\Omega)} + \langle \lambda_2(t), w(t, a) \rangle_{L^2(\Omega)} + \langle \lambda_3(t), w(t, b) \rangle_{L^2(\Omega)} \leq r,
$$

where

$$
L(w) = \|w_t + w\|_{L^2(\Omega)} + \|w(0, x) - u_0(x)\|_{L^2(\Omega)} + \|w(t, a)\|_{L^2(\Omega)} + \|w(t, b)\|_{L^2(\Omega)}
$$

$$
= \|f\|_{L^2(\Omega)} + \|g - u_0\|_{L^2(\Omega)} + \|h_1\|_{L^2(\Omega)} + \|h_2\|_{L^2(\Omega)}.
$$

for some $r > 0$. Since $\|\lambda_1(x)\|_{L^2(\Omega)}, \|\lambda_2(t)\|_{L^2(\Omega)}$ and $\|\lambda_3(t)\|_{L^2(\Omega)}$ are uniformly bounded during the training process as in [3.10] Hölder’s inequality implies that $L(w)$ should be bounded by some constant $C$ which depends only on $r$. To explain it more precisely, Hölder’s inequality yields

$$
-\|\lambda_1(x)\|_{L^2(\Omega)} \|w(0, x) - u_0(x)\|_{L^2(\Omega)} + \langle \lambda_2(t), w(t, a) \rangle_{L^2(\Omega)} + \langle \lambda_3(t), w(t, b) \rangle_{L^2(\Omega)}
$$

$$
\geq -\|\lambda_1(x)\|_{L^2(\Omega)} \|w(0, x) - u_0(x)\|_{L^2(\Omega)} - \|\lambda_2(t)\|_{L^2(\Omega)} \|w(t, a)\|_{L^2(\Omega)} + \|w(t, a)\|_{L^2(\Omega)}
$$

Note that the last equation is of first order with respect to $\|g - u_0\|_{L^2(\Omega)}$, $\|h_1\|_{L^2(\Omega)}$ and $\|h_2\|_{L^2(\Omega)}$. Since $L(w)$ contains the second order terms, the three norms should be bounded by some constant which depends only on $r$ and the desired properties are followed.
Now we consider the composition of \( w = (w - I) + I = e + I \). Then \( \|e\|_{L^2([0,T]\times\Omega)} \) is bounded by a constant depending on \( r \) due to the boundedness of three terms \( \|g\|_{L^2([0,T]\times\Omega)}, \|h_1\|_{L^2([0,T])} \) and \( \|h_2\|_{L^2([0,T])} \) with the above observation and Grönwall’s inequality. Note that \( \|I\|_{L^2([0,T]\times\Omega)} \) has the same form of upper bound by construction. In conclusion, usual triangular inequality gives the boundedness for \( \|w\|_{L^2([0,T]\times\Omega)} \), and therefore, the set \( M(r) = \{w \in L^2(\Omega) \cap \{L_\nu(w) \leq r \text{ for some } n \in \mathbb{N}\} \) is bounded in \( L^2([0,T] \times \Omega) \) for \( r > 0 \).

The set \( M(r) \) is also bounded in \( L^2([0,T]; H^1(\Omega)) \) by the above estimate. If we integrate (21) over \([0, T]\) and considering the previous discussion about the boundedness of \( \|e\|_{L^2(\Omega)} \), then the term \( \int_0^T \|\partial_x e\|^2_{L^2(\Omega)} \) should be bounded by a constant which depends only on \( r \) when \( w \in M(r) \). To derive further properties about the boundedness of \( M(r) \), we multiply the equation (20) by \( -\partial_x^2 e \). Using the integration by parts, the following holds.

\[
\frac{1}{2} \frac{d}{dt} \|\partial_x e\|^2_{L^2(\Omega)} + \nu \|\partial_x^2 e\|^2_{L^2(\Omega)} = \nu \int_{\partial\Omega} \partial_x e \partial_x e \cdot n dS + \int_{\Omega} e \partial_x \partial_x^2 e dx + \int_{\Omega} e \partial_x \partial^2 e dx + \int_{\Omega} I \partial_x e \partial_x^2 e dx - \int_{\Omega} f^* \partial_x^2 e dx.
\]

Using Morrey’s inequality and Hölder’s inequality, we can estimate the right side of equation as follows. For an arbitrary small \( \eta > 0 \),

\[
\int_{\partial\Omega} \partial_x e \partial_x e \cdot n dS = \partial_x e(t, a) \partial_x e(t, a) - \partial_x e(t, b) \partial_x e(t, a) = 0
\]
\[
\int_{\Omega} e \partial_x \partial_x^2 e dx \leq \frac{1}{4\eta} \|e\|_{L^2(\Omega)}^2 + \eta\|\partial_x^2 e\|_{L^2(\Omega)}^2 \leq \frac{1}{4\eta} \|e\|_{L^2(\Omega)}^2 + \frac{1}{4\eta} \|\partial_x^2 e\|_{L^2(\Omega)}^2
\]
\[
\int_{\Omega} I \partial_x e \partial_x^2 e dx \leq \frac{1}{4\eta} \|I\|_{L^2(\Omega)} \|\partial_x e\|_{L^2(\Omega)} \|\partial_x^2 e\|_{L^2(\Omega)} \leq \frac{1}{4\eta} \|I\|_{L^2(\Omega)} \|\partial_x e\|_{L^2(\Omega)} \|\partial_x^2 e\|_{L^2(\Omega)}
\]
\[
\int_{\Omega} f^* \partial_x^2 e dx \leq \frac{1}{4\eta} \|f^*\|_{L^2(\Omega)} \|\partial_x^2 e\|_{L^2(\Omega)} \leq \frac{1}{4\eta} \|f^*\|_{L^2(\Omega)} \|\partial_x^2 e\|_{L^2(\Omega)}.
\]

Since \( \eta > 0 \) is an arbitrary constant, we may assume that \( \nu > 8\eta \). Consequently, we can derive the following inequality.

\[
\frac{d}{dt} \|\partial_x e\|^2_{L^2(\Omega)} + \nu \|\partial_x^2 e\|^2_{L^2(\Omega)} \leq \frac{C_1}{2\eta} \|\partial_x e\|_{L^2(\Omega)}^2 + \frac{C_1}{4\eta} \|I\|_{H^1(\Omega)}^2 \|\partial_x e\|_{L^2(\Omega)}^2 + \frac{1}{4\eta} \|f^*\|_{L^2(\Omega)}^2.
\]

By the above discussion, the terms \( \|\partial_x e\|_{L^2([0,T]\times\Omega)}, \|\partial_x g^*\|_{L^2(\Omega)}, \|\partial_x I\|_{L^2(\Omega)}, \|f^*\|_{L^2(\Omega)} \) are bounded by a constant which depends only on \( r, T \) and an uniform constant \( \nu \) in the assumption. Therefore, by Grönwall’s inequality, we can conclude that there exists a constant \( c(r, T, \Omega) \) such that

\[
\sup_{0 \leq t \leq T} \|\partial_x e\|_{L^2(\Omega)} \leq \exp\left(\int_0^T \frac{C_1}{2\eta} dt\right) \left(\frac{C_1}{4\eta} \|I\|_{H^1(\Omega)}^2 dt + \int_0^T \frac{1}{4\eta} \|f^*\|_{L^2(\Omega)}^2 dt\right)
\]

Now, if we integrate the inequality (22) over \([0, T]\), the term \( \|\partial_x e(T, \cdot)\|_{L^2(\Omega)} \) should be bounded since \( \|\partial_x e(0, \cdot)\|_{L^2(\Omega)} \).

\[
\|\partial_x e(T, \cdot)\|_{L^2(\Omega)} \leq \sup_{0 \leq t \leq T} \|\partial_x e\|_{L^2(\Omega)} \|I\|_{H^1(\Omega)} \|\partial_x g^*\|_{L^2(\Omega)} + \|\partial_x I\|_{L^2([0,T]\times\Omega)} + \|\partial_x^2 e\|_{L^2([0,T]\times\Omega)} \|I\|_{H^1(\Omega)} \|\partial_x g^*\|_{L^2(\Omega)} \|I\|_{H^1(\Omega)} + \frac{1}{4\eta} \|f^*\|_{L^2(\Omega)}^2.
\]

On the one hand,

\[
\partial_t w = -w \partial_x w + \nu \partial_x^2 w + f
\]

where

\[
\|w \partial_x\|_{L^2([0,T]\times\Omega)} \leq \|\partial_x w\|_{L^2([0,T]\times\Omega)} \|w\|_{L^2([0,T]\times\Omega)} \times \|\partial_x\|_{L^2([0,T]\times\Omega)} \leq T \sup_{0 \leq t \leq T} \|\partial_x w\|_{L^2(\Omega)} \|w\|_{L^2([0,T]\times\Omega)} \leq T \left( \frac{C_1}{2\eta} \|\partial_x e\|_{L^2(\Omega)} + \|\partial_x g^*\|_{L^2(\Omega)} + \frac{1}{4\eta} \|f^*\|_{L^2(\Omega)} \right)^2.
\]

Therefore, \( \partial_t w \) lies in \( L^2([0,T] \times \Omega) \) and we can conclude that \( \|w\|_{L^2([0,T]; H^2(\Omega))} \) and \( \|\partial_t w\|_{L^2([0,T]; L^2(\Omega))} \) are bounded by a constant which depends only on \( r, T, \epsilon \).
Proof of Theorem 3.8 for Klein–Gordon equation

The Klein–Gordon equation reads:

$$\partial^2_{tt} u - \alpha \partial^2_{xx} u + \beta u + \gamma u^k = f(t, x), \quad (t, x) \in [0, T] \times \Omega$$

where $\alpha, \beta, \gamma$ are positive constants with odd number $k > 0$. We consider the case where $\Omega$ is an one dimensional interval $[0, 1]$ and $k = 3$. We assume the uniform boundedness of $\partial_x g_1^t, \partial_t h_1^t, \partial_x^2 h_1^t$ and $\partial_t h_2^*, \partial_x^2 h_2^*$ where $h_1^t, h_2^*$ and $g_1^t$ are boundary and initial conditions of the neural network solution $w$. The details are as follows.

**Assumption C.4.** There exists a constant $\epsilon > 0$ such that $\int_{[0, T]} (\partial_t g_1^t)^2 + (\partial_t h_1^t)^2 + (\partial_t^2 h_1^t)^2 + (\partial_t h_2^*)^2 + (\partial_x^2 h_2^*)^2 dt \leq \epsilon$.

**Proof.** Suppose that the neural network solution $w(t, x)$ satisfies the following.

$$\partial^2_{tt} w - \alpha \partial^2_{xx} w + \beta w + \gamma w^3 = f^*(t, x), \quad (t, x) \in [0, T] \times \Omega$$

$$w(0, x) = g_1^t(x), \quad x \in \Omega$$

$$\partial_t w(0, x) = g_2^t(x), \quad x \in \Omega$$

$$w(t, a) = h_1^t(t), w(t, b) = h_2^t(t), \quad t \in [0, T]$$

We again consider the interpolation function $I(t, x) = h_1(t)(1 - x) + h_2(t)x$. Note that the norms of $I(t, x), \partial_t I(t, x)$ and $\partial_t^2 I(t, x)$ are bounded by a constant multiple of $\sum_{0 \leq a \leq 2} ||\partial_x^a h_1||_{L^2([0, T])} + ||\partial_x^a h_2||_{L^2([0, T])}$ in $L^2([0, T]; H^2(\Omega))$. Furthermore, the integrability of the square of nonlinear term $I(t, x)^k$ can be found as follows by using Morrey’s inequality.

$$\int_{[0, T] \times \Omega} I^{2k}(t, x) dt dx \leq ||I||_{L^{\infty}([0, T] \times \Omega)}^{2k-2} ||I||_{L^2([0, T] \times \Omega)}^{2} \leq C_1 ||I||_{L^2([0, T] \times \Omega)}^{2k-2} ||I||_{L^2([0, T] \times \Omega)}^{2}$$

where $C_1$ is a constant depending only on $T$. On the other hand, Morrey’s inequality yields that there exists a constant $C$ such that

$$h_1(0), h_2(0) \leq ||h_1||_{L^\infty([0, T])} + ||h_2||_{L^\infty([0, T])} \leq C ||h_1||_{H^1([0, T])} + ||h_2||_{H^1([0, T])}$$

$$\partial_t h_1(0), \partial_t h_2(0) \leq ||\partial_t h_1||_{L^\infty([0, T])} + ||\partial_t h_2||_{L^\infty([0, T])} \leq C ||h_1||_{H^1([0, T])} + ||h_2||_{H^1([0, T])}.$$ 

Thus, we can conclude that $u(0, x) - I(0, x)$ should be contained in $L^2(\Omega)$ with $u(0, 0) - I(0, 0) = u(0, 1) - I(0, 1) = 0$. Let $e(t, x) := w(t, x) - I(t, x)$. Now we estimate the terms in the equation below.

$$\partial^2_{tt} e - \alpha \partial^2_{xx} e + \beta e + \gamma(3I^2e + 3Ie^2 + e^3) = f^{**}, \quad (t, x) \in [0, T] \times \Omega,$$

$$e(0, x) = g_1^*(x), \quad x \in \Omega,$$

$$\partial_t e(0, x) = g_2^*(x), \quad x \in \Omega,$$

$$e(t, a) = 0, e(t, b) = 0, \quad t \in [0, T],$$

where

$$f^{**}(t, x) = f^*(t, x) - (\partial^2_{tt} I + \alpha \partial^2_{xx} I - \beta I - \gamma I^3)$$

$$g_1^*(x) = g_1^t(x) - g_1^t(0)(1 - x) - g_1^t(1)x,$$

$$g_2^*(x) = g_2^t(x) - g_2^t(0)(1 - x) - g_2^t(1)x.$$ 

Note that the $L^2$ norms of $g_1^{**}, g_2^{**} \in L^2(\Omega)$ and $f^{**} \in L^2([0, T] \times \Omega)$ are bounded by $||g_1||_{L^2(\Omega)}, ||g_2||_{L^2(\Omega)}, ||f||_{L^2(\Omega)}$ and $||\partial_x^a h_i||_{L^2([0, T])}$ through the above discussion involving Morrey’s inequality. Let us define the functional $E(u)$ as below.

$$E(u) = \int_{\Omega} |\partial_t e|^2 + \alpha |\partial_x e|^2 + \beta |e|^2 + \gamma |e|^4 dx.$$
Then, the following holds due to the fact that \( e \) is sufficiently differentiable.

\[
\frac{1}{2} \frac{d}{dt} E(u) = \int_{\Omega} \partial_t^2 e \partial_t e + \alpha \partial_t e \partial_t \partial_x e + \beta e \partial_t e + \gamma e^3 \partial_t e \, dx \\
= \int_{\Omega} \partial_t^2 e \partial_t e - \alpha \partial_t^2 e \partial_t \partial_x e + \beta e \partial_t e + \gamma e^3 \partial_t e \, dx - \int_{\partial \Omega} \partial_x e \partial_t e \cdot ndS \\
= \int_{\Omega} (f^{**} - (3I^2 e + 3I^2 e^2)) \partial_t e \, dx.
\]

With Young’s inequality and Hölder’s inequality, we can bound the three terms on the right hand side.

\[
\int_{\Omega} f^{**} \partial_t e \, dx \leq \frac{1}{2} |f^{**}|_{L^2(\Omega)}^2 + \frac{1}{2} \int_{\Omega} |\partial_t e|^2 \, dx \\
\int_{\Omega} I^2 e \partial_t e \, dx \leq \int_{\Omega} I^2 e^2 \, dx + \frac{1}{4} \int_{\Omega} |\partial_t e|^2 \, dx \leq \int_{\Omega} e^2 \, dx + \frac{1}{4} \int_{\Omega} |\partial_t e|^2 \, dx \\
\int_{\Omega} I e^2 \partial_t e \, dx \leq \int_{\Omega} I e^2 \, dx + \frac{1}{4} \int_{\Omega} |\partial_t e|^2 \, dx \leq \|I\|_{L^\infty(\Omega)} \int_{\Omega} e^2 \, dx + \frac{1}{4} \int_{\Omega} |\partial_t e|^2 \, dx
\]

Consequently, we have the following inequality.

\[
\frac{d}{dt} E(u) \leq (1 + \frac{3}{2} \gamma + \|I\|_{L^\infty(\Omega)}) E(u) + \frac{3}{4} \|I\|_{L^2(\Omega)}^2 + \|f^{**}\|_{L^2(\Omega)}
\]

Finally, Grönwall’s inequality implies that

\[
\sup_{0 \leq t \leq T} E(u) \leq (1 + \frac{3}{2} \gamma + \|I\|_{L^\infty(\Omega)}) E(u) + \frac{3}{4} \|I\|_{L^2(\Omega)}^2 + \|f^{**}\|_{L^2(\Omega)}
\]

Note that \( \int_0^T \|I\|_{L^\infty(\Omega)}^2 \) can be bounded by a constant multiple of \( \|h_1\|_{H^2([0, T])}^2 + \|h_2\|_{H^2([0, T])}^2 \) by the above discussion with Morrey’s inequality. The Poincaré inequality yields an upper bound of \( \|g_1^{**}\|_{L^4(\Omega)}^2 \) which is a constant multiple of \( \|g_1^{**}\|_{H^1(\Omega)}^2 \). Now we suppose that the neural network \( w \) such that \( L_n(w) \leq r \) for some \( n \in \mathbb{N} \). That is,

\[
L_n(w) = L(w) + (\lambda_1(x), w(0, x) - g_1(x))_{L^2(\Omega)} + (\lambda_2(t), w(0, x) - g_2(x))_{L^2(\Omega)} \\
+ (\lambda_3(t), w(t, a) - h_1(a))_{L^2(\Omega)} + (\lambda_4(t), w(t, b) - h_2(b))_{L^2(\Omega)} \\
\leq r,
\]

where

\[
L(w) = \|f - f^{**}\|_{L^2([0, T] \times \Omega)}^2 + \|g_1 - g_1^{**}\|_{L^2(\Omega)}^2 + \|g_2 - g_2^{**}\|_{L^2(\Omega)}^2 + \|h_1 - h_1^{**}\|_{L^2(\Omega)}^2 + \|h_2 - h_2^{**}\|_{L^2(\Omega)}^2.
\]

for some \( r > 0 \). If we develop similar arguments as before, we can conclude that the set \( \{ w \in L^2(\Omega) | L_n(w) \leq r \} \) for some \( n \in \mathbb{N} \) should be bounded in \( H^{1,1}([0, T] \times \Omega) \).

\[\square\]

**Theorem 3.9.** Consider a sequence of quasi-minimizers \( \{u_n\}_{n \in \mathbb{N}} \) with respect to \( \{L_n\}_{n \in \mathbb{N}} \). Then, \( u_n \rightharpoonup u \) in the weak topology, where \( u \) is the minimizer of functional \( L \) (i.e., \( u \) is the solution of equation (11)). This holds for the Helmholtz (10), viscous Burgers (19), and Klein–Gordon equations (23).

**Proof.** We begin with showing that \( u \in L_A \). Let us suppose otherwise, \( u \) is not a function satisfying \( T(u) = g \) in \( L^2(\partial \Omega) \). The trace operator \( T \), which is a bounded and linear operator, admits an adjoint operator \( T^* : H^1(\Omega) \rightarrow L^2(\partial \Omega) \). This implies that \( T(u_n) \rightarrow T(u) \neq g \) weakly, whenever \( u_n \rightarrow u \) in the weak sense from the standard argument below.

\[
\langle T(u_n) - T(u), v \rangle_{L^2(\partial \Omega)} = \langle T(u_n - u), v \rangle_{L^2(\partial \Omega)} \\
= \langle u_n - u, T^*(v) \rangle_{H^1_0(\Omega)}.
\]
Consequently, we obtain the following contradiction by the Cauchy–Schwarz inequality with Lemma 3.10

\[ \lim_{m \to \infty} \inf_{n=1}^{m} \langle T(u_n) - g, T(u) - g \rangle_{L^2(\partial \Omega)} = \lim_{m \to \infty} \inf_{n=1}^{m} \langle \sum_{n=1}^{m} T(u_n) - mg, T(u) - g \rangle_{L^2(\partial \Omega)} \]

\[ \leq \lim_{m \to \infty} \sup_{n=1}^{m} \| \sum_{n=1}^{m} T(u_n) - mg \|_{L^2(\partial \Omega)} \| T(u) - g \|_{L^2(\partial \Omega)} < \infty. \]

Now we assume that \( u \in L_A \), for a sequence \( \{u_n\}_{n \in \mathbb{N}} \) with \( u_n \to u \). The convexity of the mapping \( x \mapsto |x|^2 \) yields the inequality

\[ \| T(u_n) - g \|^2_{L^2(\Omega)} \geq \| T(u) - g \|^2_{L^2(\Omega)} + 2 \langle T(u) - g, T(u) - T(u_n) \rangle_{L^2(\Omega)}, \]

where \( \langle T(u) - g, T(u) - T(u_n) \rangle_{L^2(\Omega)} \to 0 \) by the weak convergence. By the Cauchy–Schwarz inequality,

\[ \langle \lambda_n, T(u_n) - g \rangle_{L^2(\partial \Omega)} \geq -\| \lambda_n \|_{L^2(\partial \Omega)} \cdot \| T(u_n) - g \|_{L^2(\partial \Omega)}, \]

and therefore, we obtain the following inequality by the boundedness of \( \| \lambda_n \|_{L^2(\partial \Omega)} \) with the lower semi-continuity of \( L^2(\partial \Omega) \) norm.

\[ L(u) = \| Nu - f \|_{L^2(\Omega)} \leq \liminf_{n \to \infty} (\| Nu_n - f \|^2_{L^2(\Omega)} + \beta \| T(u_n) - g \|^2_{L^2(\partial \Omega)} + \langle \lambda_n, Tu_n - g \rangle_{L^2(\partial \Omega)}) \]

\[ = \liminf_{n \to \infty} L_n(u_n) \]

Next, we prove that a recovery sequence exists. For a given sequence \( \{\lambda_n\}_{n \in \mathbb{N}} \) and \( u \in L_A \), a sequence \( \{u_n\}_{n \in \mathbb{N}} \) that satisfies the following inequality holds in \( A_n \).

\[ \limsup_{n \to \infty} L_n(u_n) \leq L(u). \]

If \( u \notin L_A \), consider any sequence \( \{u_n\}_{n \in \mathbb{N}} \) in \( A_n \). Since \( F(u) = \infty \), it is obvious that the above inequality holds. Conversely, suppose that \( u \in L_A \). By Theorem 3.3, there exists a sequence \( \{u_n\}_{n \in \mathbb{N}} \) in \( A_n \) such that \( \| Nu - Nu_n \|_{V(\Omega)} < 1/n \). Then \( \{u_n\}_{n \in \mathbb{N}} \) is a desired sequence since \( T(u_n) \to T(u) \) in \( L^2(\partial \Omega) \) by the continuity of the trace operator so that

\[ \limsup_{n \to \infty} L_n(u_n) = \limsup_{n \to \infty} (\| Nu_n - f \|^2_{L^2(\Omega)} + \beta \| T(u_n) - g \|^2_{L^2(\partial \Omega)} + \langle \lambda_n, Tu_n - g \rangle_{L^2(\partial \Omega)}) \]

\[ \leq \limsup_{n \to \infty} (\| Nu - f \|^2_{L^2(\Omega)} + 1/n) = L(u). \]

In conclusion, \( u_n \to u \) weakly in \( H^1(\Omega) \) by Theorem 3.3. One the one hand, by Rellich-embedding theorem from \( W^{1,2} \) to \( L^2 \), the embedding of \( H^1(\Omega) \) into \( L^2(\Omega) \) is a compact operator so that it maps weakly convergent sequence to strongly convergent sequence. Therefore, \( u_n \to u \) in \( L^2(\Omega) \) strongly.

**Lemma 3.10.** Consider a sequence of quasi-minimizers \( \{u_n\}_{n \in \mathbb{N}} \) with respect to \( \{L_n\}_{n \in \mathbb{N}} \) for a sufficiently large \( \beta \). Then, the corresponding \( \| \lambda_n \|_{L^2(\partial \Omega)} \) is bounded for all \( n \in \mathbb{N} \).

**Proof.** For an arbitrary small \( \varepsilon > 0 \), there exists a neural network with width \( n \in \mathbb{N} \) such that \( \| Nu - f \|_{L^2(\Omega)} < \varepsilon \) by Theorem 3.5. Since trace operator is continuous, \( \| Tu_n - Tg \|^2_{L^2(\partial \Omega)} = \| Tu_n - Tu \|^2_{L^2(\partial \Omega)} \) is also bounded by a constant multiple of \( \varepsilon \). Then, by the definition of quasi-minimizer,

\[ L_n(u_n) \leq \beta \| Tu_n - g \|^2_{L^2(\partial \Omega)} + \langle \lambda_n, Tu_n - g \rangle_{L^2(\partial \Omega)} \]

\[ \leq \delta_n + O(\varepsilon). \]
We have,
\[ \|\lambda_{n+1}\|_{L^2(\partial \Omega)} = \langle \lambda_{n+1}, \lambda_{n+1} \rangle_{L^2(\partial \Omega)} \]
\[ = \langle \lambda_n + \eta_n(Tu_n - g), \lambda_n + \eta_n(Tu_n - g) \rangle_{L^2(\partial \Omega)} \]
\[ = \langle \lambda_n, \lambda_n \rangle_{L^2(\partial \Omega)} + 2\eta_n \langle \lambda_n, Tu_n - g \rangle_{L^2(\partial \Omega)} + \eta_n^2 \langle Tu_n - g, Tu_n - g \rangle_{L^2(\partial \Omega)} \]
\[ \leq \|\lambda_n\|_{L^2(\partial \Omega)} + 2\eta_n \delta_n + (\eta_n^2 - 2\eta_n \beta)\|Tu_n - g\|^2_{L^2(\partial \Omega)} \]

Therefore, if \( \beta \) is sufficiently large so that \( \beta > \frac{1}{\delta}(\eta_n + \frac{2\delta_n}{\|Tu_n - g\|^2_{L^2(\partial \Omega)}}) \) for all \( n \in \mathbb{N} \), then \( \{\|\lambda_n\|_{L^2(\partial \Omega)}\}_{n \in \mathbb{N}} \) is a decreasing sequence. In conclusion, \( \{\lambda_n\} \) must be a bounded sequence in \( L^2(\partial \Omega) \).

\[\square\]

**Trace Theorem for the viscous Burgers and Klein–Gordon equations**

To generalize the discussions in Theorem 3.9 and Lemma 3.10 to the viscous Burgers and Klein–Gordon equations, we need the continuity of the trace operators. For a complete explanation, we introduce some definitions and theorems. For a function \( u(t, x) : [0, T] \times \Omega \to \mathbb{R} \) with \( u(t_1, \cdot) \in H^2(\Omega) \) for every \( t_1 \in [0, T] \), \( u : [0, T] \to H^2(\Omega) \) is defined by \( u(t) := u(t, x) \).

Let \( u' : [0, T] \to H(\Omega) \) be a function satisfying
\[ \int_0^T \phi'(t)u(t)dt = -\int_0^T \phi(t)u'(t)dt \]
for every \( \phi(t) \in C^\infty_c([0, T]) \). Then, the following holds.

**Theorem C.5** (Thm 4 in Sec 5.9 of Evans (1998)). Suppose that \( \Omega \) is a open and bounded with smooth boundary \( \partial \Omega \). For \( u \in L^2([0, T]; H^2(\Omega)) \) and \( u' \in L^2([0, T]; L^2(\Omega)) \), there exists a constant \( C(T, \Omega) \) such that
\[ \max_{0 \leq t \leq T} \|u(t)\|_{H^1(\Omega)} \leq C(T, \Omega)(\|u\|_{L^2([0, T]; H^2(\Omega))} + \|u'\|_{L^2([0, T]; L^2(\Omega))}) \]

Motivated by the above theorem, we can extend the trace theorem to the equation with the Dirichlet boundary condition. Consider the case when a spatial domain is an interval \([0, 1] \subseteq \mathbb{R} \). Then, the following holds.

**Corollary C.6.** For \( u \in L^2([0, T]; H^2(\Omega)) \) and \( u' \in L^2([0, T]; L^2(\Omega)) \), let us define boundary functions \( h_1, h_2 : [0, T] \to \mathbb{R} \) and a initial function \( g : \Omega \to \mathbb{R} \) by
\[ h_1(t) := \text{trace}(u(t))(0), h_2(t) := \text{trace}(u(t))(1) \text{ and } g(x) := u(0). \]

where \( \text{trace} : W^{1,2}(\Omega) \to L^2(\partial \Omega) \) denotes the trace operator. Then, there exists a constant \( C \) depending only on \( T, \Omega \) such that the following inequality holds.
\[ \|h_1(t)\|_{L^2([0, T])} + \|h_2(t)\|_{L^2([0, T])} + \|g(x)\|_{L^2(\Omega)} \leq C(\|u\|_{L^2([0, T]; H^2(\Omega))} + \|u'\|_{L^2([0, T]; L^2(\Omega))}). \]

**Proof.** Let us denote the constant in the theorem C.5 by \( C(T, \Omega) \). Then, we can estimate \( \|g(x)\|_{L^2(\Omega)} \) as follows.
\[ \|g(x)\|_{L^2(\Omega)} \leq \|g(x)\|_{H^1(\Omega)} \leq \max_{0 \leq t \leq T} \|u(t)\|_{H^1(\Omega)}. \]

On the one hand, we can estimate other two terms applying the usual trace theorem.
\[ \|h_1(t)\|_{L^2([0, T])} + \|h_2(t)\|_{L^2([0, T])} \leq T \max_{0 \leq t \leq T}(h_1(t) + h_2(t)) \leq \sqrt{2TC_{\text{trace}}} \max_{0 \leq t \leq T} \|u(t)\|_{H^1(\Omega)}. \]

where \( C_{\text{trace}} \) denotes a constant in the trace theorem which depends only on \( \Omega \), not on \( t \). Combining two inequalities, we get the desired property.

\[\square\]

For the Klein–Gordon equation, we introduce the following trace theorem on a Lipschitz domain.

**Theorem C.7** (Thm 1.1 in Gagliardo (1957)). Suppose that \( \Omega \in \mathbb{R}^n \) is a bounded set with Lipschitz boundary \( \partial \Omega \). Then, there exists a bounded linear operator \( T : W^{1,p}(\Omega) \to L^p(\partial \Omega) \) and a constant \( C \) such that \( \|T(u)\|_{L^p(\partial \Omega)} \leq C\|u\|_{W^{1,p}(\Omega)} \) and,
\[ T(u) = u|_{\partial \Omega} \text{ for } u \in W^{1,p}(\Omega) \cap L^p(\Omega), \]
where \( C \) depends only on \( p \) and \( \Omega \).
Recall that we constructed the sequence $L_n(w)$ of loss functional as below for the viscous Burgers’ equation.

$$L_n(w) = L(w) + \langle \lambda_1(x), w(0, x) - u_0(x) \rangle_{L^2(\Omega)} + \langle \lambda_2(t), w(t, a) \rangle_{L^2([0,T])} + \langle \lambda_3(t), w(t, b) \rangle_{L^2([0,T])},$$

where

$$L(w) = \|w_t + w w_x - \nu w_{xx}\|_{L^2([0,T] \times \Omega)}^2 + \beta \|w(0, x) - u_0(x)\|_{L^2(\Omega)}^2 + \beta \|w(t, a)\|_{L^2([0,T])}^2 + \beta \|w(t, b)\|_{L^2([0,T])}^2.$$

Define a function $\lambda : [0, T] \times \{0\} \cup \{0\} \times \Omega \cup [0, T] \times \{1\}$ by

$$\lambda(t, 0) = \lambda_2(t), \lambda(t, 1) = \lambda_3(t) \text{ and } \lambda(0, x) = \lambda_1(x), \forall t \in [0, T], x \in \Omega.$$

Then, update rules for $\lambda_1, \lambda_2$, and $\lambda_3$ during the training can be transformed into an update rule for $\lambda$. In this setting, we can apply all of the previous arguments to prove Theorem 3.9 and Lemma 3.10 for the viscous Burgers’ equation.