An Orthogonal Neural Network-Based Extreme Learning Machine Approach for Solving Linear Chemical Physics Differential Equations

Raksha B. Patel[1], Priyanka N. Thorat[2], Divyesh V. Chavda[3]

[1]*Department of Chemistry, Government Arts Commerce and Science College Khergam*
[2]*Department of Physics, Government Arts Commerce and Science College Khergam*
[3]*Department of Mathematics, Government Arts Commerce and Science College Khergam*
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Abstract—**Differential equations are fundamental in chemistry and physics, especially in areas such as chemical physics, governing processes including diffusion, heat trans- fer, electrostatics, and reaction-transport. Although some equations are linear, explicit analytical solutions do not exist due to complex geometries, varied mate- rial properties, and nontrivial boundary conditions, which frequently make data unavailable. This paper presents an Orthogonal neural network-based Extreme Learning Machine (ONN-ELM) numerical framework for approximating solutions to linear differential equations with boundary conditions. The hidden layers are re- placed by a single-layer functional expansion block, and to optimize weights, we use the ELM algorithm. The proposed approach provides a mesh-free, computationally efficient, and physically consistent alternative to traditional numerical methods**

Index Terms—**Linear differential equations, orthogonal neural network-based extreme learn- ing machine, chemical physics, numerical approximation, physics-based learning**

I. INTRODUCTION

Differential equations form the mathematical backbone of chemical physics, providing quantitative descriptions of transport, interaction, and energy transfer processes such as diffusion, heat conduction, electrostatics, and reaction–transport phenomena [1,2]. Linear partial differential equations frequently arise in these contexts and are fundamental to modeling steady-state and equilibrium systems.

Although linearity guarantees mathematical properties such as stability and unique- ness, closed- form analytical solutions are often unavailable due to complex geometries, heterogeneous material properties, and nontrivial boundary conditions. Consequently, numerical methods are commonly employed. Classical approaches such as finite difference, finite element, and finite volume methods require mesh generation, which becomes computationally expensive and difficult to implement for high-dimensional or irregular domains [3].

Recent advances in machine learning have introduced alternative, mesh-free strategies for solving differential equations. Physics-informed neural networks and related approaches have shown promising results [4]. Among these, the Extreme Learning Machine (ELM) offers a fast and analytically tractable framework due to its non-iterative training strategy [5]. This study investigates an orthogonal neural network-based ELM (ONN- ELM) for solving linear chemical physics differential equations when exact solutions are unavailable. Relevant references supporting the methodology and problem formulation are provided throughout the paper.

II. LINEAR GOVERNING EQUATION IN CHEMICAL PHYSICS

We consider a general linear partial differential equation defined over a spatial domain Ω:
$$L[u(x)] = f(x), x \in \Omega \qquad (1)$$
where $u(x)$ denotes a physical quantity such as concentration or temperature, L is a linear differential operator, and $f(x)$ is a known source term.

A representative example encountered in chemical physics is the steady-state diffusion– reaction equation:

$$-D\nabla^2 u(\mathrm{x}) + ku(\mathrm{x}) = S(\mathrm{x}) \tag{2}$$

where D is the diffusion coefficient and k is a reaction rate constant.

III. ORTHOGONAL NEURAL NETWORK-BASED EXTREME LEARNING MACHINE METHOD

3.1. Solution Approximation

In the ONN-ELM framework, the unknown solution is approximated as:

$$u(\mathbf{x}) \approx \sum_{i=1}^{N} \beta_i P_i(\mathbf{a}_i \cdot \mathbf{x}) \tag{3}$$

where $P_i(\cdot)$ is an orthogonal polynomial based activation function, w_i and b_i are randomly assigned input parameters, and β_i are output weights to be determined.

3.2. Enforcing the Differential Equation

Applying the linear operator L yields:

$$\mathcal{L}[u(\mathbf{x})] = \sum_{i=1}^{N} \beta_i \mathcal{L}[P_i(\mathbf{a}_i \cdot \mathbf{x})] \tag{4}$$

At collocation points x_j, the governing equation is enforced:

$$\sum_{i=1}^{N} \beta_i \mathcal{L}[P_i(\mathbf{a}_i \cdot \mathbf{x}] = f(\mathbf{x}_j) \tag{5}$$

3.3. Boundary Conditions

Boundary conditions of the form:

$$u(\mathrm{x}) = g_b(\mathrm{x}), \mathrm{x} \in \partial\Omega \tag{6}$$

are imposed by enforcing:

$$\sum_{i=1}^{N} \beta_i P_i(\mathbf{a}_i \cdot \mathbf{x}) = g_b(\mathbf{x}_b) \tag{7}$$

at boundary collocation points x_b.

IV. LINEAR ALGEBRAIC SYSTEM

Combining the interior and boundary equations produces a linear system:
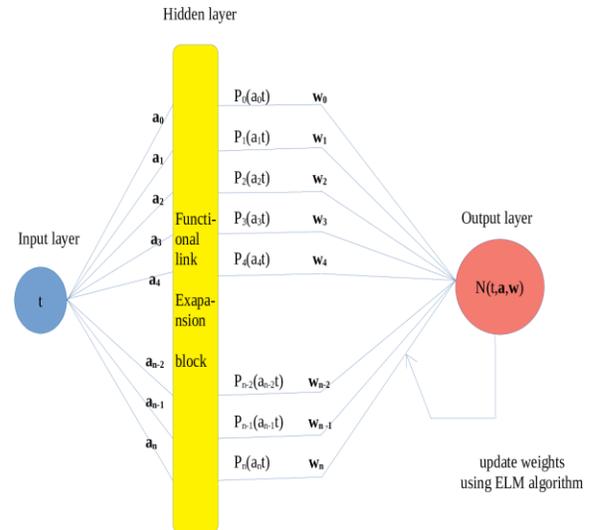
$$A\beta = \mathbf{b} \tag{8}$$

Figure 1: The structure of orthogonal neural network

which is solved analytically using the Moore–Penrose pseudoinverse:

$$\beta = \mathbf{A}^\dagger \mathbf{b} \tag{9}$$

V. NUMERICAL EXAMPLES

To demonstrate the effectiveness of the proposed Orthogonal Neural Network-Based Ex- treme Learning Machine (ONN-ELM) framework, a representative linear chemical physics problem is considered. Similar benchmark diffusion–reaction models have been widely used in the literature to validate numerical solvers [2, 4].

We consider the steady-state diffusion–reaction equation defined on the domain $0 \le x \le 1$:

$$-D\frac{d^2 u(x)}{dx^2} + ku(x) = S(x), \tag{10}$$

where $u(x)$ represents the concentration of a chemical species, D is the diffusion coeffi- cient, k is the reaction rate constant, and $S(x)$ is a prescribed source term. For numerical implementation, the parameters are chosen as

$$D = 1, k = 1, S(x) = \sin(\pi x), \tag{11}$$

subject to the Dirichlet boundary conditions

$$u(0) = 0, u(1) = 0. \tag{12}$$

In the ONN-ELM framework, the approximate solution is expressed as

$$u(x) \approx \sum_{i=1}^{N} \beta_i \, P_i(\mathbf{a}_i \cdot \mathbf{x}),$$

$$(13)$$

where $P_i(\cdot)$ denotes the orthogonal polynomial based activation function, w_i and b_i are randomly assigned input parameters, and β_i are the output weights to be determined.

Applying the differential operator yields

$$-\sum_{i=1}^{N} \beta_i \frac{d^2}{dx^2} P_i(\mathbf{a}_i \cdot \mathbf{x}) + \sum_{i=1}^{N} \beta_i P_i(\mathbf{a}_i \cdot \mathbf{x}) = \sin(\pi x).$$

$$(14)$$

The governing equation is enforced at interior collocation points, while the boundary conditions are imposed at $x = 0$ and $x = 1$. This results in a linear algebraic system of the form

$$A\beta = b, \qquad\qquad (15)$$

which is solved analytically using the Moore–Penrose pseudoinverse.

The ONN-ELM approximation is constructed using orthogonal polynomial activation functions, and the governing equation, along with boundary conditions, is enforced at collocation points. The resulting linear algebraic system is solved analytically using the Moore-Penrose pseudoinverse, as discussed in earlier sections. This example illustrates the ability of the proposed ONN-ELM framework to efficiently approximate solutions to linear chemical physics differential equations without requiring mesh generation or iterative optimization.

VI. RESULTS AND DISCUSSION

The ONN-ELM-based solution satisfies the governing linear differential equation at all collocation points and provides a smooth approximation over the computational domain. Increasing the number of hidden neurons improves accuracy while preserving numerical stability, consistent with observations reported in earlier ELM studies [5]. The proposed method avoids iterative optimization and significantly reduces computational cost com- pared to traditional numerical solvers.

VII. ADVANTAGES

The proposed approach offers several advantages:
- Mesh-free formulation
- Fast analytical training
- Compatibility with linear physical laws
- Reduced computational complexity

VIII. LIMITATIONS AND FUTURE WORK

Accuracy depends on the number and placement of collocation points. Future work may extend the method to time-dependent problems, coupled systems, and hybrid numerical– machine learning approaches.

IX. CONCLUSION

This study demonstrates that Orthogonal Neural Network-Based Extreme Learning Ma- chines can effectively approximate solutions to linear chemical physics differential equa- tions when exact analytical solutions are unavailable. The approach preserves physical consistency, exploits mathematical linearity, and offers a computationally efficient alter- native to classical numerical solvers.

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