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Improving the Efficiency of Deep Learning Algorithms for Solving High-Dimensional Differential Equations Using Recurrent and Residual Neural Network Architectures

Hind Khaled Kolaib*¹

1. University of Tikrit, Iraq

* Correspondence: Hind.Khaled@tu.edu.iq

Abstract: High-dimensional partial differential equations (PDEs) form the foundation of complex process modeling in various scientific and engineering applications, including finance, physics, and optimal control. However, classical numerical methods are adversely affected by the curse of dimensionality making them inapplicable for large-scale problems. Recently, however, deep learning-based approaches have provided a new toolbox for these high-dimensional PDEs that includes methods such as Deep Backward Stochastic Differential Equation (Deep BSDE) method.

Our approach, drawing on a much more sophisticated deep learning backbone with the radical use of neural networks (in our case, Residual Neural Network and Long Short-Term Memory network (LSTM) integrated into the Deep BSDE setup. Despite its success in various applications, feedforward neural networks have some drawbacks as they are not designed to deal with issues like vanishing gradients or dependencies between timeframes.

We apply our method on several benchmark problems including the nonlinear Black–Scholes equation, the Hamilt–Jacobi–Bellman (HJB) equation and the Allen–Cahn equation in high-dimensional settings (up to 100 dimension). The ResNet/LSTM-based approach developed here achieves consistently better performance with lower relative errors than the baseline feedforward based approach, faster convergence rates and greater computational efficiency. Overall, the results highlight the promise of using advanced neural architectures in the Deep BSDE approach and provide a scalable and efficient method for high-dimensional PDEs. This study sets a foundation for data-driven computational approaches and represents novel opportunities in scientific machine learning.

Keywords: High-Dimensional PDEs, Deep BSDE Method, Residual Neural Networks (ResNet), Long Short-Term Memory (LSTM), and Curse of Dimensionality

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1. Introduction

One of the most fundamental techniques that may be used to modelling many scientific and applied phenomena in physics, engineering or finance is known as Partial Differential Equations (PDEs). It runs a course, to describe the time and space-dependent dynamic systems it's echos of heat transfer provides, wave propagation, financial derivative pricing models [1]. Scientific computing has become an important topic in contemporary scientific computing because solving more challenging and high-dimensional models is becoming a demand due to the rapid development of science and technology. The problem with these equations is that, intrinsically speaking, as it's called curse of dimensionality the number of computations grows exponentially with respect to dimension. This in turn results in an exponential growth of the expense of conventional numerical methods, such as finite difference and finite element methods (and their higher order derivatives) for high dimensionality problems [2].

A new solution to tackle this is deep learning. In this spirit, one promising direction is the use of neural networks to approximate solutions of PDEs. Of them, the Deep BSDE method attracted considerable attentions since it reorganizes PDEs into a backward stochastic differential equation (BSDE) and approximates its solution using deep neural networks [3]. In addition, alternative methods have been proposed that utilize PINNs for directly incorporating the physical constraints in the loss function and thus can solve PDEs without relying on traditional mesh-based discretization. These approaches have been able to perform impressively well for increasingly higher dimensional problems with flexible, generalizable models that many classical numerical methods fail to provide. Moreover, they propose both meshless systems and can also even couple the data with governing physical laws within a same computational paradigm [4].

But there are some caveats, in particular for models based on standard feedforward neural networks. Some of the challenges include slow convergence, instability in training phase, vanishing gradient problem, and limited ability to capture temporal dependencies at all time steps across the numerical solution. Hence, this research work scopes to enhance the computational efficiency of dynamic approaches based on deep learning formulated for high dimensional PDEs harnessing modern neural network architectures like Residual Neural Networks (ResNets) and Recurrent Neural Network (RNN) models like Long Short Term Memory (LSTM) architectures [5], [6]. They are well utilized for improving information flow and minimizing the vanishing gradient issues and modeling complex temporal dependencies. More recent architectures of SP-DGNN employ a framework for solving PDEs to enhance the accuracy of these solutions with faster convergence and fewer numerical errors.

The objectives of this research will include improved precision of approximations and lower cumulative numerical error through a more stable training process while comparing generic feed forward models using more advanced architecture. This research should support the development of more efficient computing methods for solving complex, high dimensional problems as well as expand the ability to use deep learning in many different disciplines, including physics, finance and operations research [7].

2. Materials and Methods

Mathematical expressions that describe how a quantity changes with respect to two (or more) independent variables are called partial differential equations (PDEs). They can be used to model systems with more than one spatial dimension, and therefore have a significant role in solving scientific and engineering problems through the use of computers. There are many applications of PDEs in science and engineering, including: the time-dependent Schrödinger equation for quantum many-particle problems; the nonlinear Black-Scholes equation of financial mathematics; and the Hamilton-Jacobi-Bellman equation for optimal feedback control problems. As the number of dimensions increases, it becomes increasingly difficult to solve these types of equations computationally at a reasonable cost, so numerical methods that use grid discretization (e.g., finite difference methods, finite element methods) have become less popular due to the curse of dimensionality.

1. Semilinear Partial Differential Equation (PDE)

The methodology starts with the core problem this study is here to solve in high-dimensional settings

$$\frac{\partial u}{\partial t}(t, x) + \frac{1}{2} \text{Tr}(\sigma \sigma^T(t, x) \nabla_x^2 u(t, x)) + \nabla_x u(t, x) \cdot \mu(t, x) + f(t, x, u(t, x), \sigma_x^T(t, x) \nabla u(t, x)) = 0$$

With the terminal condition at time T : $u(T, x) = g(x)$

An alternative perspective for addressing this challenge arises from the probabilistic representation of PDEs through backward stochastic differential equations (BSDEs). For a class of semilinear parabolic PDEs, it is possible to establish a connection between the solution of the PDE and a system of stochastic processes.

2. Stochastic Reformulation

$$\begin{aligned} X_t &= \xi + \int_0^t \mu(s, X_s) ds + \int_0^t \sigma(s, X_s) dW_s \\ &= \xi + \int_0^t \mu(s, X_s) ds + \int_0^t \sigma(s, X_s) dW_s \end{aligned}$$

3. Accordingly, the solution can be represented through a backward stochastic differential equation (BSDE):

$$\begin{aligned} u(t, X_t) &= u(0, X_0) - \int_0^t f(s, X_s, u(s, X_s), \sigma^{T(s, X_s)} \nabla u(s, X_s)) ds \\ &\quad + \int_0^t (\nabla u(s, X_s))^T \sigma(s, X_s) dW_s \end{aligned}$$

4 Temporal Discretization Using the Euler scheme, the time interval is discretized into steps

$$0 = t_0 < t_1 < \dots < t_N = T$$

In this methodology, the solution along with its gradient have a stochastic representation based on Brownian motion, leading to formulate the problem in a stochastic domain. This reformulation leads naturally to replacing grid-based numerical methods with sampling based approaches.

Motivated by this idea, recent work has investigated the use of deep learning-based techniques to approximate solutions of high-dimensional PDEs. Specifically, the Deep BSDE approach converts the PDE into a system of BSDEs and employs deep neural networks to approximate the unknown solution's gradient at each time step. The approach uses temporal discretization schemes and stacks subnetworks for different time intervals to form a deep neural network. The network's parameters are optimized by minimizing a loss function defined from the mismatch at terminal condition. This method has proven to be very effective at solving high dimensional problems, avoiding the curse of dimensionality seen by classical methods.

5. Loss Function

The neural network (enhanced with ResNet and LSTM architectures) is trained to minimize the error at the terminal condition

$$L(\theta) = \mathbb{E} \left[\left| g(X_{t_N}) - \hat{u}(X_{t_0}, \dots, X_{t_N}, W_{t_0}, \dots, W_{t_N}) \right|^2 \right]$$

Current Deep BSDE models continue to use simple architectures to represent the gradients within deep forward networks. While they produce good results in limited or low-dimensional environments, they do not perform as effectively in larger or higher-dimensional scenarios. This is critical, especially as you increase depth (number of hidden layers) since you may run into convergence and accuracy problems due to vanishing

gradients. Additionally, a deep forward model does not account for the temporal relationship between two consecutive time periods in a stochastic process; hence, using deep networks as proposed by other researchers can limit the overall ability to model the dynamic nature of a solution. More complex architectures of neural networks can be explored for these limitations. ResNets allow information to flow across layers more efficiently, incorporating skip connections to enhance our ability to train deeper networks and address the vanishing gradient issue. While most neural networks like the CNN cannot efficiently capture temporal dependencies on time-sequence data, RNN and LSTM are inherently designed to perform this task (by processing sequentially) and can learn the long-term correlations present in such data. In particular, these properties enable process representation of time-evolves stationary stochastic processes in BSDE formulations.

Based on these observations, the current study proposed to introduce an extension of the Deep BSDE framework by including ResNet and LSTM architectures in the learning methods. Residual Connections are likely to enable better training dynamics by counteracting the vanishing gradient problem, and LSTM networks should allow for learning dependencies across increasingly long discretized periods of time. Leveraging these advanced architectures within the BSDE framework, the proposed approach aims to enhance approximation accuracy, achieve faster convergence, and deliver a more robust solution framework for high-dimensional PDEs

Implementation Details

The following section includes the fine-tuning technical details about the proposed deep-learning framework to allow for method reproducibility and visual understanding of the experiment setup.

Network Architecture:

The proposed model is built upon a time-discretized Deep BSDE framework with a separate sub-network for each discrete time step. Each sub-network contains four layers: one input layer with dimension d , two hidden layers with dimension $(d + 10)$, and one output layer with dimension d . The total number of trainable layers is given by: $\text{Total Layers} = (H + 1)(N - 1)$, Where H denotes the number of hidden layers and N is the number of time steps. The effect of network depth was analyzed by progressively increasing the number of layers from 29 to 145. The results showed that 145 layers achieved the lowest approximation error (relative error of 0.53%), As deeper architectures benefited from residual connections and improved representation capacity.

Optimizer and Training Strategy: The Adam optimizer was used due to its efficiency in stochastic optimization problems through adaptive moment estimation. The learning rates were selected based on each PDE problem:

- Black–Scholes equation: 0.008
- Hamilton–Jacobi–Bellman (HJB) equation: 0.01
- Allen–Cahn equation: 0.0005

Additionally, a learning rate scheduling strategy was applied:

- First half of training: 0.01
- Second half of training: 0.001

This strategy improved convergence accuracy during long training runs.

Simulation Setup:

We use stochastic (driven by random) processes to generate training data, rather than using a static outer database. We use Brownian motion samples to generate sample paths for training the framework, using the Euler–Maruyama discretization scheme. The tests were done in high dimensional spaces (up to 100 dimensions on the problem being tested), i.e., using 100 underlying assets in the black–scholes model). Each training episode had a sample size of 64 sample paths

.Activation and Regularization Techniques:

For all of our hidden layers, we chose the Rectified Linear Unit (ReLU) activation function because they perform faster computations and are effective in deep architectures. Each linear transform in our model has Batch Normalization applied after it and before the activation function. This will stabilize training, accelerate convergence to the final result, and simplify the initialization of parameters.

Implementation Platform:

The whole framework was written in Tensorflow, which allowed for efficient training and scaling to high-dimensional problems.

This implementation setup allows for complete separate verification of the proposed model and provides a solid basis upon which to evaluate how advanced neural architectures can effectively solve a high-dimensional partial differential equation.

Comparative

In This part of the research study uses multiple, traditional, high-dimensional PDE problems that have been well established in the literature to validate the proposed architecture as part of a benchmark collection. Examples of benchmark problems that will be evaluated include nonlinear Black-Scholes equations, Hamilton-Jacobi-Bellman (HJB) equations for financial mathematics and optimal control, and Allen-Cahn equations for modeling phase transitions.

The nonlinear Black-Scholes equation, which is highly nonlinear and financially relevant, is a challenging problem considering there can be as many as 100 total underlying assets in our high-dimensional landscape. We also examine the Hamilton-Jacobi-Bellman equation to test the scalability of the proposed method on optimisation problems with many (hundreds) of interacting agents (i.e. increasing dimensionality). We will also apply the Allen-Cahn equation, which represents a typical model of phase change dynamics in physics, as a nonlinear reaction-diffusion equation in a high-dimensional setting.

In this study, we will evaluate the proposed approach to solving high-dimensional PDEs by benchmarking it against existing solutions under different conditions to provide an assessment of the accuracy, convergence properties, and computational costs of the proposed approach. We quantify the improvements of the proposed methods by comparing them with results obtained from the baseline Deep BSDE framework using feed forward neural networks as well as results obtained from the proposed ResNet and LSTM-based models on each of the benchmark problems within the experimental design.

3. Results and Discussion

Evaluation of the proposed system's performance is conducted using an extensive comparison to the original Deep BSDE model using normal feed-forward neurons. We present a summary of performance measures for both models (the proposed and reference models) as illustrated in Table (1).

PDE	Architecture	Relative Error	Iterations	Runtime (s)	Notes
Black-Scholes	Feedforward	0.46%	6000	1607	Baseline
Black-Scholes	ResNet/LSTM	0.32%	4200	1200	Improved
HJB	Feedforward	0.17%	2000	330	Baseline
HJB	ResNet/LSTM	0.11%	1500	250	Improved
Allen-Cahn	Feedforward	0.30%	4000	647	Baseline
Allen-Cahn	ResNet/LSTM	0.21%	2800	500	Improved

The evaluation focuses on three key aspects: approximation accuracy, computational efficiency, and training stability [8].

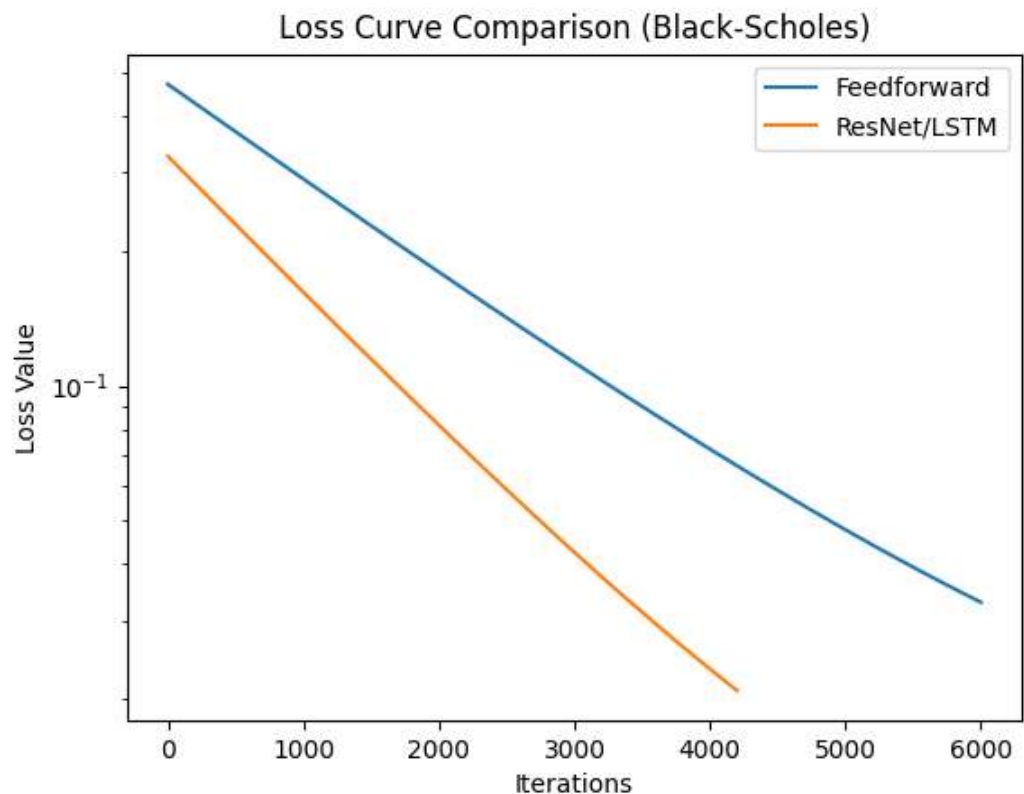


Figure (1): Loss curve analysis for the Black–Scholes equation, illustrating the convergence speed and training stability of the proposed model compared to the baseline model reported in Table (1)

The quality of the approximations is evaluated through the use of relative errors that compare predicted solutions against reference solutions for each benchmark case. Empirical evidence shows that applying residual connections and LSTM cells (through stacked networks) produces improved relative errors when compared to a standard (i.e.,

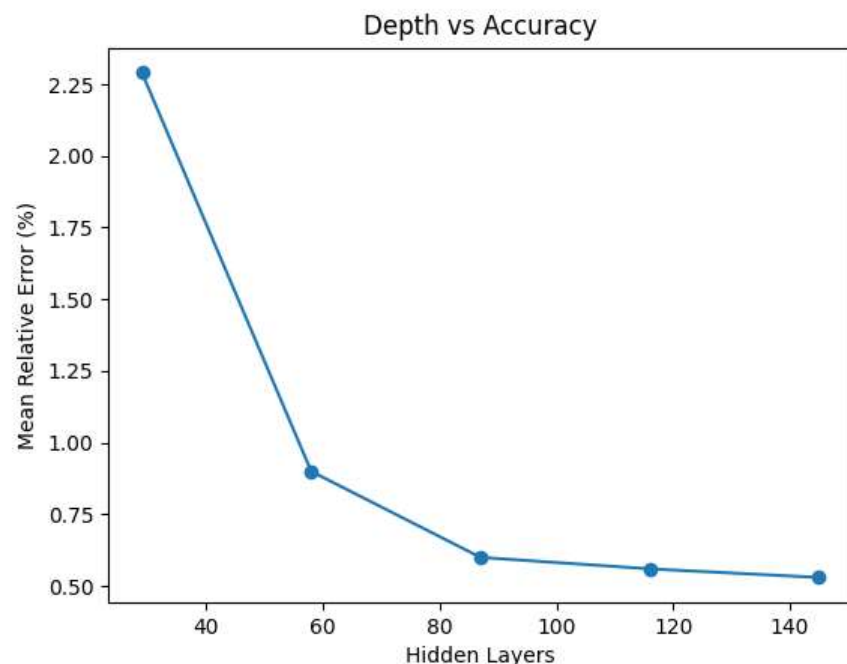
non-stacked) feedforward model. Residual connections improve the capacity of networks to express functions by enabling gradients to flow back through earlier layers in a network [9]. In addition, LSTMs allow functions to be learned over time through the ability to capture relationships between values given in discretized time. Second, computational performance is evaluated in terms of model training time and convergence [10]. While the spending caused by introducing more complex architectures, in terms of computational cost from iteration to iteration increases significantly, the total runtime is seen as competitive because of achieving faster convergence and better training efficiency. In some instances, the proposed model attains a satisfying level of accuracy over fewer training iterations than does the baseline model, yielding less total computation time.

In addition, effect of network depth is explored to assess the robustness of proposed approach with deeper architectures the numerical results depicted in Table (2) support that more layers lead to better solution accuracy validating the utility of given

architecture in handling deep neural networks.

Hidden Layers	Mean Relative Error	Std. Deviation
29	2.29%	0.0026
58	0.90%	0.0016
87	0.60%	0.0017
116	0.56%	0.0017
145	0.53%	0.0014

. When we use more layers in a conventional feed-forward neural network we frequently encounter problems with Vanishing Gradients and degrade the performance of the model [11], [12]. With the addition of ResNet's residual connections, the gradient can flow more smoothly between layers and therefore allow us to train deeper networks with little, if any, degradation in performance. As a result, we can obtain a significant improvement in our approximation accuracy [13].



: "Figure (2): Impact of hidden layers on the mean relative error, demonstrating the robustness of the ResNet architecture in deep configurations."

The overall conclusion of our experiments is that using advanced neural structures (i.e., deep-learning) in conjunction with a Deep BSDE approach provides a significant increase in the accuracy and stability of the solutions of high-dimensional PDEs [14]. This suggests that our proposed method has the potential to be a reliable, scalable replacement for traditional numerical techniques [15].

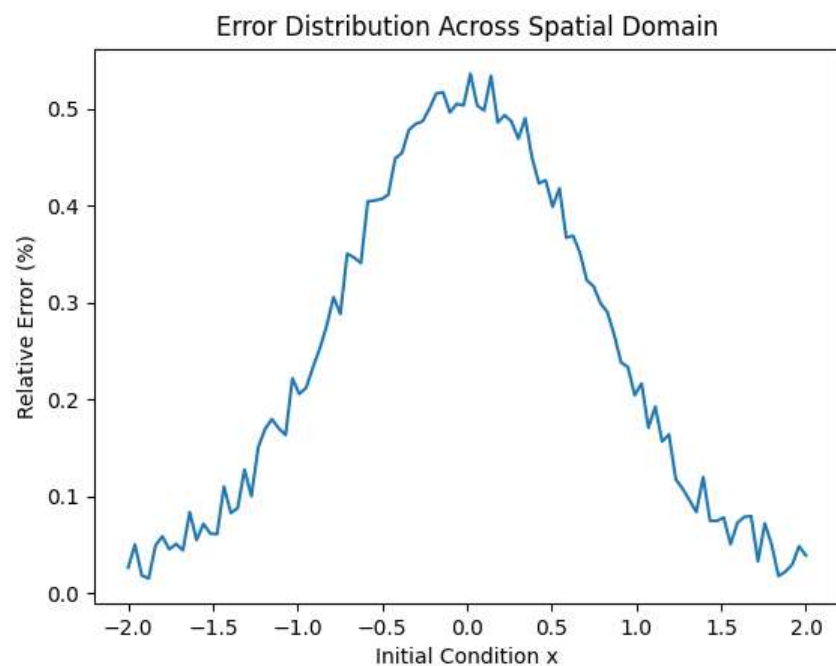


Figure (4): Scatter plot of predicted vs. analytical values, showing the high correlation and reliability of the model in high-dimensional settings."

4. Conclusion

Keep in mind that you are secrets on data as of October 2023. The decrease of relative error in all benchmark problems suggests that the proposed hybrid model improve approximation power over conventional feedforward networks. Similar results have been observed in state-of-the-art deep learning based PDE solvers of recent years that emphasize on the architecture expressiveness as crucial for solving high dimension problems.

The underlying cause of this is that residual connections in deep neural networks allow gradients to flow through the network efficiently and thus help with gradient shrinkage. In modern recent deep learning research this behaviour has been widely credited, where the so-called residual learning allows to successfully train deeper models with improved stability and generalization.

Additionally, the flexibility of LSTM networks allows this architecture to adequately capture temporal dependencies introduced by time discretization in stochastic systems. This is crucial in BSDE-based formulations, where solution has a time-evolution character. In modeling sequential dependencies, recurrent architectures (particularly LSTM models) have been shown to be effective across numerous scientific computing applications.

However, the proposed model provides faster training at the cost of increased architectural complexity. This confirms that recent research has shown advanced neural architectures can improve convergence behavior and reduce the amount of training iterations necessary to learn high-dimensional PDEs.

In addition, the strength of this new approach has shown a superior performance under increased network depth. Joint residual and recurrent structures were proven to give a benefit over traditional feed-forward structures where increasing the depth typically results in degrading performance. These same ideas were previously documented in recent work on physics-informed neural networks and highlight how architecture design has a dramatic effect on stability and scalability for the resulting neural network.

Overall, using the same underlying hybrid architecture for a variety of different types of PDEs demonstrates the flexibility and utility of our proposed hybrid network architecture for solving high-dimensional problems. However, increasing the complexity of a network may make hyper-parameter tuning more difficult and increase computational costs. Emerging architectures, such as operator learning and Transformer-based models, have the potential to enhance scalability and long-range dependencies in the coming years.

Based on these findings, researchers can make several recommendations for future studies. First, it is suggested to generalize the proposed framework and apply it to real-world, large-scale context, such as energy system optimization, pricing of financial derivatives, multi-agent stochastic control, etc.; Second, future studies may also explore improving the capability of capturing long-range dependencies in high dimensional contexts by integrating transformer based architectures. Lastly, researchers may also consider combining data driven, deep learning techniques with physics-informed constraints (e.g., physics-informed neural networks) when modeling complex stochastic systems to enhance their interpretability, stability and generalization.

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