Hutchinson Trace Estimation for High-Dimensional and High-Order Physics-Informed Neural Networks

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Abstract

Physics-Informed Neural Networks (PINNs) have proven effective in solving partial differential equations (PDEs), especially when some data are available by blending seamlessly data and physics. However, extending PINNs to high-dimensional and even high-order PDEs encounters significant challenges due to the computational cost associated with automatic differentiation in the residual loss function calculation. Herein, we address the limitations of PINNs in handling high-dimensional and high-order PDEs by introducing the Hutchinson Trace Estimation (HTE) method. Starting with the second-order high-dimensional PDEs, which are ubiquitous in scientific computing, HTE is applied to transform the calculation of the entire Hessian matrix into a Hessian vector product (HVP). This approach not only alleviates the computational bottleneck via Taylor-mode automatic differentiation but also significantly reduces memory consumption from the Hessian matrix to an HVP's scalar output. We further showcase HTE's convergence to the original PINN loss and its unbiased behavior under specific conditions. Comparisons with the Stochastic Dimension Gradient Descent (SDGD) highlight the distinct advantages of HTE, particularly in scenarios with significant variability and variance among dimensions. We further extend the application of HTE to higher-order and higher-dimensional PDEs, specifically addressing the biharmonic equation. By employing tensor-vector products (TVP), HTE efficiently computes the colossal tensor associated with the fourth-order high-dimensional biharmonic equation, saving memory and enabling rapid computation. The effectiveness of HTE is illustrated through experimental setups, demonstrating comparable convergence rates with SDGD under memory and speed constraints. Additionally, HTE proves valuable in accelerating the Gradient-Enhanced PINN (gPINN) version as well as the Biharmonic equation. Overall, HTE opens up a new capability in scientific machine learning for tackling high-order and high-dimensional PDEs.

1   Introduction

Physics-Informed Neural Networks (PINNs) [44] have made significant strides in solving partial differential equation (PDE) problems in scientific computing, particularly for low-dimensional equations. This is attributed to their powerful fitting capability [34], generalization [36], and stability in optimization [37]. However, despite the demonstrated capacity of neural networks in modeling high-dimensional data in image and text domains, PINNs' exploration of high-dimensional and high-order PDEs has been relatively limited. The primary challenge arises from the enormous computational cost involved in the automatic differentiation process of calculating the residual loss function steps for high-dimensional and high-order PDEs under the PINNs framework.

Solving problems related to high-dimensional PDEs is crucial, considering the curse-of-dimensionality, which is prevalent in various fields such as the Black-Scholes equation in mathematical finance for option pricing, the Hamilton-Jacobi-Bellman (HJB) equation in optimal control, and the Schrödinger equation in quantum physics. Despite the availability of specialized high-dimensional PDE solvers for different domains, such as DeepBSDE [16] and Deep Splitting Method [1] for high-dimensional parabolic equations and specific algorithms for the Hamilton-Jacobi equation [13, 14], a unified and effective approach for solving *general* high-dimensional PDEs is lacking.

PINNs is a versatile method capable of handling arbitrary PDEs and being mesh-free, in principle it is not susceptible to the curse-of-dimensionality. Despite recent efforts to use PINNs for solving high-dimensional PDEs, such as Stochastic Dimension Gradient Descent (SDGD) [22] and random smoothing [18, 23], these approaches have their limitations. SDGD attempts to reduce each stochastic gradient's computational cost and memory consumption by sampling dimensions. However, when significant variability and variance among dimensions exist, SDGD's stochastic gradients may suffer from substantial variance, hindering convergence. As for random smoothing methods, they smooth the original neural network with Gaussian noise, impacting the network's expressive power and making it less effective in handling non-smooth PDE solutions.

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To address the limitations of PINN in tackling high-dimensional and even high-order PDEs, herein, we propose the use of Hutchinson Trace Estimation (HTE) [25] to accelerate PINNs and reduce memory cost. HTE can be applied to various common PDEs, such as second-order parabolic equations and the biharmonic equation. Firstly, for second-order parabolic PDEs, the computational bottleneck lies in the need to calculate the entire Hessian, with its computational cost increasing quadratically with the dimensionality. HTE is seamlessly integrated into the PINNs framework to alleviate this central computational bottleneck. Specifically, HTE transforms the calculation of the entire Hessian matrix into a Hessian vector product (HVP). Unlike the full Hessian, which is a large matrix of dimensions $d \times d$, where d is the dimensionality of the PDE problem, the output of HVP is a scalar, significantly reducing memory consumption. Moreover, HVP can efficiently utilize Taylor-mode automatic differentiation [7] in JAX [8] for rapid computation, achieving both acceleration and reduced memory usage.

Furthermore, we demonstrate that the loss of PINNs with HTE converges to the original version of PINN loss under certain conditions and is unbiased, providing a solid foundation for its convergence properties. We also discuss the distinctions, similarities, and applicability between HTE and SDGD, the most related methodologies. We present examples illustrating when HTE or SDGD is more suitable and how their variances depend on the PDE problem. After addressing second-order parabolic equations, we explore how HTE is even more efficient in higher-order and higher-dimensional scenarios, motivating the extension of HTE to the biharmonic equation.

Given that the biharmonic equation is a fourth-order high-dimensional equation, attempting to solve it directly with conventional PINNs would lead to a massive tensor of size d^4, where d represents the dimensionality of the PDE problem, and 4 denotes the order of the equation. However, by extending the Hessian Vector Product (HVP) in HTE to a tensor-vector product (TVP), we can transform the computation of the entire colossal tensor into a scalar which is the TVP output. This not only saves a considerable amount of memory but also facilitates rapid computation using Taylor-mode differentiation. We also demonstrate that the extended HTE method provides an unbiased estimate for the biharmonic operator, and we analyze the sources of its variance. To emphasize the importance of properly implementing the HVP and TVP in the proposed HTE method in JAX, we present a pseudocode to familiarize readers with HTE and its efficient implementation.

Ultimately, we showcase the effectiveness of HTE in various experimental setups. Firstly, we demonstrate that HTE and SDGD exhibit similar convergence rates under the same memory constraints and speed limitations on a second-order nonlinear anisotropic parabolic equation. Notably, they successfully scale PINNs to a very high dimension (100,000 dimensions). Secondly, we illustrate how HTE can accelerate the more accurate Gradient-Enhanced PINN (gPINN). Since gPINN requires additional first-order derivatives of the original PINN residual, the computational load is substantial, but HTE mitigates this burden while keeping the improvement brought by gPINN. Lastly, we highlight the advantages of HTE in the context of higher-order, high-dimensional biharmonic equations.

This paper is arranged as follows. We present related work in Section 2. Then, we introduce the proposed HTE method in Section 3. We present computational experiments in Section 4 and summarize the paper in Section 5.

2 Related Work

Hutchinson Trace Estimation. Hutchinson Trace Estimation (HTE) [25] is an unbiased estimator of the trace of a matrix, which was first proposed for the influence matrix related to the Laplacian smoothing splines computation. Since its initial publication, progress has been made for improvement. Hutch++ [39] reduces the variance of HTE by employing a low-rank approximation methodology, whose complexity is proved to be optimal among all matrix-vector query-based methods for trace estimation. Later, Persson et al. [42] adopted the Nyström approximation to improve Hutch++ further; [48] provided a modern analysis of the HTE's error. Roosta et al. [46] proved an improved estimation for the sample efficiency in HTE. In modern deep learning, HTE has also been applied to the Diffusion model [49] to infer the probability density function of the model, where HTE can reduce the computation cost when dealing with the Jacobian of the Diffusion model, which can be a convolutional neural network or even a Transformer [50], whose derivative is extremely costly. To the best of our knowledge, we are the first to apply HTE for efficient physics-informed neural networks (PINNs) computations for high-order PDEs and in high-dimensions.

Efficient Automatic Differentiation. To implement HTE efficiently, we adopt the Taylor-mode automatic differentiation (AD) [7] in JAX [8], which is tailored for high-order AD. Indeed, the type of AD affects the speed and memory cost significantly, and the commonly used stacked forward/backward modes of AD are much slower. In addition to the superior Taylor-mode AD, other attempts exist to avoid the costly high-order derivatives. Randomized smoothing [18, 23] randomly smooths the model using Gaussian noises for inference, and its derivatives can be simulated via Monte Carlo simulation. The generalization ability of a randomly smoothed model can be interpreted by the information bottleneck theory [35]. Randomized AD [41] incorporated stochastic gradient descent (SGD) to accelerate and avoid the need for full AD.

High-Dimensional PDE Solver. Several works have considered high-dimensional PDE solvers. In [51], the significance of L^∞ loss and adversarial training in addressing high-dimensional Hamilton-Jacobi-Bellman equations

was demonstrated. The separable PINNs approach in [12] employs a structure that allows the residual points to be a tensor product of per-dimension points, thereby increasing the batch size. Nevertheless, when confronted with problems surpassing ten dimensions, memory usage becomes a serious bottleneck. DeepBSDE [16, 17] and its extensions [2, 10, 19, 24, 31, 6] are grounded in the classical BSDE interpretation for specific high-dimensional parabolic PDEs, leveraging deep learning models to approximate the unknowns in the BSDE formulation. The deep splitting method [1] unifies the splitting method with deep neural networks. Chen et al. [11] solved forward and inverse problems of Fokker-Planck equations, including Brownian noise and Levy noise in high dimensions using PINNs. FBSNN [44] established a connection between high-dimensional parabolic PDEs and forward-backward stochastic differential equations, employing deep neural networks to learn the unknown solution. The multilevel Picard methods [3, 4, 5, 26, 27] represent a nonlinear extension of Monte Carlo capable of solving parabolic PDEs under specific constraints. In [52, 53], tensor neural networks were proposed, adopting a separable structure for efficient numerical integration in solving high-dimensional Schr"odinger equations. More recently, SDGD [22] emerged as a method designed to sample dimensions in PDEs, aiming to scale up and accelerate high-dimensional PINNs. Randomized smoothing [18, 23] adopts the smoothed model with Gaussian noise so that Monte Carlo can simulate its inference and derivatives to combat the curse of dimensionality and avoid the costly automatic differentiation in high-order and high dimensions.

Physics-Informed Machine Learning. The methodology developed in this paper is based on the concept of Physics-Informed Machine Learning [33], especially Physics-Informed Neural Networks (PINNs) [45]. PINNs model and approximate the PDE solution by neural networks as surrogate models, which are trained through the boundary and residual losses. These approaches are shown theoretically to discover the underlying solutions governed by the PDEs [21, 40, 47]. PINNs have been successful in numerous fields in science and engineering [9, 15, 54, 30], and effective PINNs variants have been proposed to deal with different applications and problem settings [20, 28, 29, 32, 43].

3 Proposed Method

3.1 Preliminaries

This paper focuses on employing Physics-Informed Neural Networks (PINNs) to address high-dimensional and high-order Partial Differential Equation (PDE) problems. Additionally, it introduces the Hutchinson Trace Estimation (HTE) to accelerate PINN and reduce its memory consumption. Below, we provide an introduction to PINNs and HTE.

Physics-Informed Neural Networks (PINNs). This paper focuses on employing PINNs [45] solving partial differential equations (PDEs) defined on the domain $\Omega \subset \mathbb{R}^d$ with the boundary/initial condition on Γ and the residual condition within Ω:

$$\mathcal{B}u(\boldsymbol{x}) = B(\boldsymbol{x}) \text{ on } \Gamma, \qquad \mathcal{L}u(\boldsymbol{x}) = g(\boldsymbol{x}) \text{ in } \Omega, \tag{1}$$

Given the boundary points $\{\boldsymbol{x}_{b,i}\}_{i=1}^{n_b} \subset \Gamma$ and the residual points $\{\boldsymbol{x}_{r,i}\}_{i=1}^{n_r} \subset \Omega$, PINNs minimize the discrepancy in the residual and on the boundary:

$$\begin{aligned}
\mathcal{L}(\theta) &= \lambda_b \mathcal{L}_b(\theta) + \lambda_r \mathcal{L}_r(\theta) \\
&= \frac{\lambda_b}{n_b} \sum_{i=1}^{n_b} |\mathcal{B}u_\theta(\boldsymbol{x}_{b,i}) - B(\boldsymbol{x}_{b,i})|^2 + \frac{\lambda_r}{n_r} \sum_{i=1}^{n_r} |\mathcal{L}u_\theta(\boldsymbol{x}_{r,i}) - g(\boldsymbol{x}_{r,i})|^2,
\end{aligned} \tag{2}$$

where λ_b and λ_r are the boundary and residual loss weights, respectively.

Hutchinson Trace Estimation (HTE). The trace of a matrix $A \in \mathbb{R}^{d \times d}$ can be randomly estimated as follows:

$$\text{Tr}(A) = \mathbb{E}_{\boldsymbol{v} \sim p(\boldsymbol{v})} \left[\boldsymbol{v}^{\text{T}} A \boldsymbol{v} \right], \tag{3}$$

for all random variable $\boldsymbol{v} \in \mathbb{R}^d$ such that $\mathbb{E}_{\boldsymbol{v} \sim p(\boldsymbol{v})}[\boldsymbol{v}\boldsymbol{v}^T] = I$. Therefore, the trace can be estimated by Monte Carlo:

$$\text{Tr}(A) \approx \frac{1}{V} \sum_{i=1}^{V} \boldsymbol{v}_i^{\text{T}} A \boldsymbol{v}_i, \tag{4}$$

where each $\boldsymbol{v}_i \in \mathbb{R}^d$ are $i.i.d.$ samples from $p(\boldsymbol{v})$.

There are several viable choices for the distribution $p(\boldsymbol{v})$ in HTE, such as the most common standard normal distribution. However, to minimize the variance of HTE, we opt for the Rademacher distribution as follows: for each dimension of the vector $\boldsymbol{v} \sim p(\boldsymbol{v})$, it is a discrete probability distribution that has a 50% chance of getting +1 and a 50% chance of getting -1. The proof for the minimal variance is given in [48].

3.2 HTE for High-Dimensional Second-Order Parabolic PDEs

In this subsection, we introduce the second-order parabolic equation under consideration. Subsequently, we elaborate on how the HTE technique is seamlessly incorporated into the PINNs framework, facilitating accelerated convergence and reduced memory consumption. Following this, we delve into the theoretical properties of the HTE loss functions. Lastly, we discuss the efficient implementation of HTE, providing a JAX [8] pseudocode for HTE to aid readers in realizing its efficiency.

We focus on a class of second-order parabolic equations, which include the Fokker-Planck equation in statistical mechanics, the Black-Scholes equation in mathematical finance, the Hamilton-Jacobi-Bellman equation in optimal control, Schrödinger equation in quantum physics, etc., all ubiquitous in science and engineering:

$$\partial_t u(\boldsymbol{x}, t) + \mathrm{Tr}\left(\sigma\sigma^{\mathrm{T}}(\boldsymbol{x}, t)\left(\mathrm{Hess}_{\boldsymbol{x}}\, u\right)(\boldsymbol{x}, t)\right) + f(\boldsymbol{x}, t, u, \nabla_{\boldsymbol{x}} u) = 0, \quad \boldsymbol{x} \in \mathbb{R}^d, t \in [0, T], \tag{5}$$

where $u(\boldsymbol{x}, t)$ is the unknown exact solution we wish to solve, $\mathrm{Hess}_{\boldsymbol{x}}\, u$ denotes the Hessian matrix of u, $\sigma(\boldsymbol{x}, t) \in \mathbb{R}^{d \times d}$ is a known matrix-valued function, and $f(\boldsymbol{x}, t, u, \nabla_{\boldsymbol{x}} u)$ is also a known scalar function. PDEs with this form are of great interest in high-dimensions addressing the curse-of-dimensionality; see [1, 16, 22, 23, 44]. PINN's memory and speed bottleneck are traces of the second-order Hessian part, which is high-dimensional and high-order. Concretely, the computational cost of automatic differentiation in PINNs increases exponentially with the order [7]. Regarding dimensionality, for second-order parabolic equations, the size of the Hessian matrix increases quadratically with the dimension, making high dimensionality and high-order the primary computational bottlenecks.

To overcome the speed and memory bottleneck due to the Hessian trace, we can use the Hutchinson Trace Estimation (HTE) to estimate the trace in the equation for efficient PINNs since computing Hessian-Vector Product (HVP) is much faster and more memory-efficient than the full Hessian. The memory cost of HTE is significantly smaller than that of full PINNs and full Hessian since the output of HTE is a scalar, which reduces to $O(1)$ memory cost compared to the $O(d^2)$ in the full Hessian.

More specifically, the residual loss of the original PINN [44] on a point $(\boldsymbol{x}, t)$ is

$$L_{\mathrm{PINN}}(\theta) = \frac{1}{2}\left[\mathrm{Tr}\left(A_\theta(\boldsymbol{x}, t)\right) + B_\theta(\boldsymbol{x}, t)\right]^2, \tag{6}$$

where $A_\theta(\boldsymbol{x}, t) := \sigma\sigma^{\mathrm{T}}(\boldsymbol{x}, t)\left(\mathrm{Hess}_{\boldsymbol{x}}\, u\right)(\boldsymbol{x}, t) \in \mathbb{R}^{d \times d}$ and $B_\theta(\boldsymbol{x}, t) := \partial_t u(\boldsymbol{x}, t) + f(\boldsymbol{x}, t, u, \nabla_{\boldsymbol{x}} u) \in \mathbb{R}$.

The loss of the HTE replaces the Hessian trace part with a stochastic trace estimator:

$$L_{\mathrm{HTE}}(\theta; \{\boldsymbol{v}_i\}_{i=1}^V) = \frac{1}{2}\left(\frac{1}{V}\sum_{i=1}^V \boldsymbol{v}_i^{\mathrm{T}} A_\theta(\boldsymbol{x}, t)\boldsymbol{v}_i + B_\theta(\boldsymbol{x}, t)\right)^2, \tag{7}$$

where we adopt an HTE with batch size V, i.e., we sample $\{\boldsymbol{v}_i\}_{i=1}^V$ which are $i.i.d.$ samples from the distribution $p(\boldsymbol{v})$ such that $\mathbb{E}_{\boldsymbol{v} \sim p(\boldsymbol{v})}[\boldsymbol{v}\boldsymbol{v}^{\mathrm{T}}] = I$, which we consider the Rademacher distribution to minimize its variance [48].

Although HTE is an unbiased trace estimator, the HTE loss in equation (7) is biased due to the nonlinear mean square error loss function, which breaks the linearity of mathematical expectation, i.e., the HTE loss in equation (7) is biased while it converges to the exact PINN loss almost surely (a.s.) as $V \to \infty$. To correct the bias, similar to the techniques in Hu et al. [23], we are required to sample two sets of samples:

$$L_{\mathrm{HTE,\ unbiased}}(\theta; \{\boldsymbol{v}_i, \hat{\boldsymbol{v}}_i\}_{i=1}^V) = \frac{1}{2}\left(\frac{1}{V}\sum_{i=1}^V \boldsymbol{v}_i^{\mathrm{T}} A_\theta(\boldsymbol{x}, t)\boldsymbol{v}_i + B_\theta(\boldsymbol{x}, t)\right)\left(\frac{1}{V}\sum_{i=1}^V \hat{\boldsymbol{v}}_i^{\mathrm{T}} A_\theta(\boldsymbol{x}, t)\hat{\boldsymbol{v}}_i + B_\theta(\boldsymbol{x}, t)\right), \tag{8}$$

where $\{\boldsymbol{v}_i\}_{i=1}^V$ and $\{\hat{\boldsymbol{v}}_i\}_{i=1}^V$ are $2V$ $i.i.d.$ samples from the distribution $p(\boldsymbol{v})$. The properties of the two loss functions are summarized in the following theorem.

Theorem 3.1. *The loss $L_{HTE}(\theta)$ in equation (7) converges almost surely (a.s.) to the exact PINN loss $L_{PINN}(\theta)$ in equation (6), as $V \to \infty$, i.e.,*

$$\mathbb{P}\left(\lim_{V \to \infty} L_{HTE}(\theta; \{\boldsymbol{v}_i\}_{i=1}^V) = L_{PINN}(\theta)\right) = 1. \tag{9}$$

The loss $L_{HTE,\ unbiased}(\theta)$ in equation (8) is an unbiased estimator for the exact PINN loss $L_{PINN}(\theta)$ in equation (6), i.e.,

$$\mathbb{E}_{\{\boldsymbol{v}_i, \hat{\boldsymbol{v}}_i\}_{i=1}^V}\left[L_{HTE,\ unbiased}(\theta; \{\boldsymbol{v}_i, \hat{\boldsymbol{v}}_i\}_{i=1}^V)\right] = L_{PINN}(\theta). \tag{10}$$

Proof. The proof is presented in Appendix A.1. □

In HTE, there exists a bias-variance tradeoff as in the Randomized Smoothing PINNs in [23], where the biased version (equation (7)) involves fewer samples, resulting in lower variance, while the unbiased version (equation (8)) employs more samples, leading to excessive variance. In practice, we utilize the biased version as it proves sufficient. This is attributed to the negligible bias of HTE in practical applications if V is large enough, whose bias is much less obvious than the bias in Randomized Smoothing PINN considered in [23]. HTE's convergence results are already satisfactory. Indeed, HTE loss converges to the exact PINN loss, so its bias is negligible if V is large enough.

To conclude this subsection, we provide an implementation of HTE in a few lines of code using JAX [8]. Although HTE is mathematically formulated as an HVP, the implementation details significantly impact its speed and memory usage. For instance, a straightforward computation of the entire Hessian followed by a vector multiplication will not yield any efficiency gains. Below, we show a sample code for highly efficient HTE in JAX Taylor-mode autodiff, based on fully forward mode [7], which is super fast due to the absence of backward mode autodiff. Specifically, given an

```python
import jax
import jax.experimental.jet as jet

def hte(fn: Callable, V: int = 16) -> Callable:

  def trace_fn(x, key):
    dim = x.shape[-1]  # dimension of input
    rand_rademacher_vec = 2 * (
        jax.random.randint(key, shape=(V, dim), minval=0, maxval=2) - 0.5
    )
    taylor_mode_ad = lambda v: jet.jet(
      fun=fn, primals=(x,), series=((v, jnp.zeros(dim)),)
    )
    _, (_, hvps) = jax.vmap(taylor_mode_ad)(rand_rademacher_vec)
    return jnp.mean(hvps)

  return trace_fn
```

input function fn, we return its HTE, $\frac{1}{V} \sum_{i=1}^{V} \boldsymbol{v}_i (\text{Hess fn}) \boldsymbol{v}_i$, to estimate its Hessian trace.

3.3 Comparison with SDGD: Variance and Applicability

Recently, the related work of SDGD [22] has demonstrated robust capabilities in tackling high-dimensional PDEs and the curse-of-dimensionality. SDGD primarily relies on sampling dimensions to mitigate the computational and memory burdens associated with increasing dimensions. In contrast, HTE employs HVP to avoid the challenges posed by computing the full Hessian, whose cost grows quadratically with dimensionality. In this subsection, we will compare their variances and discuss their similarity and applicability.

3.3.1 SDGD as a Special Case of HTE

We show that SDGD can be regarded as a special case of HTE. Consider the discrete distribution $p(\boldsymbol{v})$ such that $\boldsymbol{v} = \sqrt{d} \boldsymbol{e}_i$ for $i = 1, 2, \cdots, d$ with probability $1/d$, where $\boldsymbol{e}_i$ denotes the standard basis vector with a one in the ith coordinate and zero elsewhere. Then, $\mathbb{E}_{\boldsymbol{v} \sim p(\boldsymbol{v})}[\boldsymbol{v} \boldsymbol{v}^{\mathrm{T}}] = I$, and the corresponding estimator is $\text{Tr}(A) \approx \frac{d}{|I|} \sum_{i \in I} A_{ii}$ where $I \subset \{1, 2, \cdots, d\}$ is a multiset and $|I|$ denotes its cardinality, which is exactly sampling dimensionality as SDGD. Despite the theoretical similarity, SDGD differs in the following aspects:

- To minimize gradient variance, SDGD employs sampling without replacement, meaning each dimension is selected at most once. On the other hand, if we consider SDGD as a special case of HTE, it uses sampling with resampling, i.e., a dimension can be sampled several times; thus, the sampled dimension indices, denoted as I, form a multiset instead of a set in the original SDGD formulation.

- While SDGD can be considered a special case of HTE, implementing SDGD using HTE is inefficient. This is because the probability distribution in this context takes values in a sparse vector, where most elements are zero. Optimization for sparse vectors can be applied in this scenario. However, HTE is generally implemented using non-sparse vectors, and this advantage cannot be fully exploited in this specific case.

3.3.2 Variance Comparison between HTE and SDGD

Both SDGD and HTE can speed up and scale up PINNs in high-dimensional and high-order PDEs. However, their source of variance differs due to various sampling and estimations. Specifically, we focus on the second-order parabolic PDE given in equation (5), and SDGD and HTE estimate the trace of 2nd-order derivatives $\mathrm{Tr}(A) = \sum_{i=1}^{d} A_{ii}$, where $A = \sigma\sigma^{\mathrm{T}}(\boldsymbol{x}, t)(\mathrm{Hess}_{\boldsymbol{x}} u)(\boldsymbol{x}, t)$. For simplicity, we drop A's dependency on $\theta, \boldsymbol{x}, t$. In the following theorems and their corresponding remarks, we prove the variance of SDGD and HTE and explain their various sources.

Theorem 3.2. *Given the SDGD estimator of the trace $\mathrm{Tr}(A) \approx \frac{d}{B}\sum_{i \in I} A_{ii}$ given an index set $I \subset \{1, 2, \cdots, d\}$ whose cardinality $|I| = B$, where B is the SDGD's batch size for the dimension, its variance is*

$$\mathbb{V}\left[\frac{d}{B}\sum_{i \in I} A_{ii}\right] = \frac{1}{\binom{d}{B}}\left(\sum_{I:|I|=B}\frac{d}{B}\sum_{i \in I} A_{ii} - \sum_{i=1}^{d} A_{ii}\right)^2, \tag{11}$$

where $\binom{d}{B} = \frac{d(d-1)\cdots(d-B+1)}{B(B-1)\cdots 1}$.

Proof. The proof is presented in Appendix A.3. □

Remark 1. *SDGD's variance comes from the variance between diagonal elements across different dimensions.*

Theorem 3.3. *Given the HTE estimator of the trace $\mathrm{Tr}(A) \approx \frac{1}{V}\sum_{k=1}^{V} \boldsymbol{v}_k^{\mathrm{T}} A \boldsymbol{v}_k$, where V is the HTE batch size and each dimension of $\boldsymbol{v}_k \in \mathbb{R}^d$ is an i.i.d. sample from the Rademacher distribution, then its variance is $\frac{1}{V}\sum_{i \neq j} A_{ij}^2$.*

Proof. The proof is presented in Appendix A.4. □

Remark 2. *HTE's variance only comes from the off-diagonal elements.*

Based on this observation, the following statements can be inferred:

- If the diagonal elements are similar, i.e., the PDE exact solution is symmetric, then SDGD has low variance.

- If the off-diagonal elements of the Hessian are zero, i.e., different dimensions do not interact, then HTE is exact.

- If the scales of off-diagonal elements are much larger than the diagonal ones, then HTE suffers from huge variance.

Hence, we propose the following examples to showcase when HTE or SDGD can outperform each other and when they perform similarly:

- **SDGD fails but HTE is accurate**. Consider the 2D exact solution $f(x, y) = -kx^2 + ky^2$ and its Laplacian $\Delta f(x, y) = 0$, where $k \in \mathbb{R}^+$ is large enough. For SDGD, we choose the batch size of dimension as 1. Thus, the estimator of SDGD will either be $\frac{\partial^2 f(x,y)}{\partial x^2} = -2k$ or $\frac{\partial^2 f(x,y)}{\partial y^2} = 2k$, whose variance is $4k^2$. For HTE, since the off-diagonal elements in the Hessian matrix of f are zero, HTE is exact, i.e., has zero variance. In brief, for this case, SDGD suffers from the variance $4k^2$ when k is large, while HTE's variance is zero.

- **HTE fails but SDGD is accurate**. Consider the 2D exact solution $f(x, y) = kxy$ and its Laplacian $\Delta f(x, y) = 0$, where $k \in \mathbb{R}^+$ is large enough. Since the diagonal of its Hessian matrix is all zero, SDGD is exact, i.e., SDGD has zero variance since $\frac{\partial^2 f(x,y)}{\partial x^2} = \frac{\partial^2 f(x,y)}{\partial y^2} = 0$ is exact. For HTE, suppose that its batch size is $V = 1$. Then HTE's estimator is $2v_1 v_2 \frac{\partial^2 f(x,y)}{\partial x \partial y} = 2v_1 v_2 k$ where v_1 and v_2 follows the Rademacher distribution. Thus, HTE's variance is $4k^2$. In brief, for this case, HTE suffers from the variance $4k^2$ when k is large, while SDGD's variance is zero and SDGD is exact.

- **HTE and SDGD have the same nonzero variance**. Consider the 2D exact solution $f(x, y) = k(-x^2 + y^2 + xy)$ and its Laplacian $\Delta f(x, y) = 0$. For SDGD, we choose the batch size of dimension as 1. Thus, the estimator of SDGD will either be $\frac{\partial^2 f(x,y)}{\partial x^2} = -2k$ or $\frac{\partial^2 f(x,y)}{\partial y^2} = 2k$, whose variance is $4k^2$. For HTE, suppose that its batch size is $V = 1$. Then HTE's estimator is $2v_1 v_2 \frac{\partial^2 f(x,y)}{\partial x \partial y} = 2v_1 v_2 k$, where v_1 and v_2 follows the Rademacher distribution. Thus, HTE's variance is $4k^2$. In brief, HTE and SDGD have the same nonzero variance $4k^2$.

However, we emphasize that the specific use case can be much more complex. Since we are applying SDGD or HTE to the neural network at each iteration, the characteristics of the function represented by the network determine which method is superior. This, in turn, is challenging to observe directly. Therefore, we provide these insights to readers as a basis for consideration. In practical applications, SDGD and HTE algorithms can be judiciously chosen based on some *a priori* knowledge of the PDE problem and the true solution. One can explore the simultaneous application of two methods and observe the rate of training loss reduction for each. Given the strong correlation between the error in approximating the true solution by PINN and the training loss [21], algorithms with lower variance are more likely to converge faster.

3.3.3 Applicability Comparison between HTE and SDGD

Next, we move to discuss the applicability of HTE compared to SDGD. HTE is more beneficial in higher dimensions and higher orders; otherwise, regular autograd methods may already be sufficient. For instance, consider the extreme case of one dimension. In this scenario, the Hessian is just a scalar. Consequently, the computational cost and memory consumption for both HVP and the full Hessian are exactly the same, hence providing no advantage for HTE. Another example will be high-dimensional but low-order; while the HTE approach can be applied to first-order PDEs, i.e., the norm square of the Jacobian can be unbiasedly estimated by Jacobian-vector product (JVP):

$$\|\nabla_{\boldsymbol{x}} u(\boldsymbol{x})\|^2 = \mathbb{E}_{v \sim p(v)} |v^{\mathrm{T}} \nabla_{\boldsymbol{x}} u(\boldsymbol{x})|^2, \tag{12}$$

experiments indicate that memory savings are insignificant. This term $\|\nabla_{\boldsymbol{x}} u(\boldsymbol{x})\|^2$ is ubiquitous in scientific computing, e.g., the first-order Hamilton-Jacobi equation, and the Schrödinger equation in the variation form. (see section 5.4 of SDGD [22] where SDGD scales up tensor neural networks for the Schrödinger equation).

More generally, from a mathematical perspective, for a d-dimensional nth-order PDE, the pure autograd computation results in a tensor of dimensions d^n. For example, the Jacobian is of dimension d, and the Hessian is of dimension d^2. In contrast, the output of HTE are V scalars when using V as the batch size; thus, the output dimension is V. Consequently, as the dimension and order increase, the advantages of HTE become more pronounced.

3.4 Applications to Biharmonic Equations

Given that HTE demonstrates superior performance for high-order and high-dimensional PDEs, we illustrate its application to the biharmonic equation in this subsection. The biharmonic equation is a fourth-order PDE that can be defined in any dimension. We will demonstrate how to extend HTE, involving the generalization of HVP to a tensor-vector product, and provide a JAX pseudo-code for efficient implementation.

Concretely, the fourth-order and d-dimensional Biharmonic operator is given by

$$\Delta^2 u(\boldsymbol{x}) = \sum_{i=1}^{d} \sum_{j=1}^{d} \frac{\partial^4}{\partial \boldsymbol{x}_i^2 \partial \boldsymbol{x}_j^2} u(\boldsymbol{x}). \tag{13}$$

The biharmonic equation is crucial in understanding and simulating complex behaviors. It is a cornerstone in analyzing systems governed by higher-order differential equations, including modeling elastic membranes, thin plates, and stream functions in fluid dynamics. We will attempt to generalize HTE, starting with the extension of HVP to a tensor-vector product (TVP), to solve high-dimensional and high-order Biharmonic equations efficiently.

Theorem 3.4. *The biharmonic operator can be unbiasedly estimated using the following TVPs:*

$$\Delta^2 u(\boldsymbol{x}) = \frac{1}{3} \mathbb{E}_{\boldsymbol{v} \sim \mathcal{N}(0,I)} \left[\frac{\partial^4}{\partial \boldsymbol{x}^4} u(\boldsymbol{x}) [\boldsymbol{v}, \boldsymbol{v}, \boldsymbol{v}, \boldsymbol{v}] \right], \tag{14}$$

where $\mathcal{N}(0,I)$ is the d-dimensional unit Gaussian, and

$$\frac{\partial^4}{\partial \boldsymbol{x}^4} u(\boldsymbol{x}) \in \mathbb{R}^{d \times d \times d \times d}, \quad \text{where} \quad \left[\frac{\partial^4}{\partial \boldsymbol{x}^4} u(\boldsymbol{x}) \right]_{ijkl} = \frac{\partial^4}{\partial \boldsymbol{x}_i \partial \boldsymbol{x}_j \partial \boldsymbol{x}_k \partial \boldsymbol{x}_l} u(\boldsymbol{x}), \tag{15}$$

and the TVP is defined as

$$\frac{\partial^4}{\partial \boldsymbol{x}^4} u(\boldsymbol{x}) [\boldsymbol{v}, \boldsymbol{v}, \boldsymbol{v}, \boldsymbol{v}] = \sum_{i,j,k,l=1}^{d} \frac{\partial^4}{\partial \boldsymbol{x}_i \partial \boldsymbol{x}_j \partial \boldsymbol{x}_k \partial \boldsymbol{x}_l} u(\boldsymbol{x}) \boldsymbol{v}_i \boldsymbol{v}_j \boldsymbol{v}_k \boldsymbol{v}_l, \tag{16}$$

Proof. The proof is presented in Appendix A.2. $\square$

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Therefore, we can also obtain an unbiased estimate of the biharmonic operator through sampling. To help the reader understand the implementation of the tensor vector product, we provide a pseudocode implementation based on JAX [8] Taylor Mode automatic differentiation [7]. We want to emphasize again that the implementation details significantly impact the speed and memory usage. A straightforward computation of the entire fourth-order derivative tensor followed by the vector multiplication will not yield any efficiency gains. Rather, we should leverage Taylor-mode automatic differentiation to allow JAX to implicitly compute the Tensor-Vector Product (TVP), thereby avoiding the massive memory consumption associated with explicit calculations. Furthermore, internal optimizations within JAX can be exploited to enhance speed by directly invoking JAX's TVP functionality and extracting only the output TVP, as opposed to the entire fourth-order derivative tensor. Similar to our previous treatment of the HTE for Hessian trace

```python
import jax
import jax.experimental.jet as jet

def hte(fn: Callable, V: int = 16) -> Callable:

  def biharmonic_fn(x, key):
    dim = x.shape[-1]  # dimension of input
    rand_gaussian_vec = (
        jax.random.normal(key, shape=(V, dim))
    )
    taylor_mode_ad = lambda v: jet.jet(
      fun=fn, primals=(x,),
      series=((v, jnp.zeros(dim), jnp.zeros(dim), jnp.zeros(dim),)
    )
    _, (_, _, _, tvps) = jax.vmap(taylor_mode_ad)(rand_gaussian_vec)
    return jnp.mean(tvps)

  return biharmonic_fn
```

estimation, we analyze the HTE's variance when estimating the biharmonic operator. Here, we employ a Gaussian distribution instead of a Rademacher distribution, and thus both diagonal and off-diagonal elements contribute to a certain extent of variance. Consequently, a larger HTE batch size, denoted as V, is required when estimating the biharmonic operator.

4 Computational Experiments

4.1 Nonlinear Second-Order PDEs with Anisotropic and Inseparable Solutions

This subsection considers nonlinear second-order Sine-Gordon PDEs with anisotropic and inseparable solutions. The following complicated exact solution is considered in related work [22, 23] to test the convergence of high-dimensional PDE solvers:

$$u_{\text{exact}}(\boldsymbol{x}) = \left(1 - \|\boldsymbol{x}\|_2^2\right) \left(\sum_{i=1}^{d-1} c_i \sin(\boldsymbol{x}_i + \cos(\boldsymbol{x}_{i+1}) + \boldsymbol{x}_{i+1} \cos(\boldsymbol{x}_i))\right), \tag{17}$$

where $c_i \sim \mathcal{N}(0, 1)$. The term $1 - \|\boldsymbol{x}\|_2^2$ is multiplied for a zero boundary condition on the unit ball to prevent the boundary loss from leaking the solution's information. The solution's ith and $(i + 1)$th dimension correlate, also known as the two-body interaction.

Based on the idea, we further introduce the following complicated exact solutions to test various algorithms:

$$u_{\text{exact}}(\boldsymbol{x}) = \left(1 - \|\boldsymbol{x}\|_2^2\right) \left(\sum_{i=1}^{d-2} c_i \exp(\boldsymbol{x}_i \boldsymbol{x}_{i+1} \boldsymbol{x}_{i+2})\right), \tag{18}$$

where the three-body interaction between each pair $(\boldsymbol{x}_i, \boldsymbol{x}_{i+1}, \boldsymbol{x}_{i+2})$ is considered.

As for the nonlinear PDE, the Sine-Gordon equation with zero boundary condition is considered

$$\Delta u(\boldsymbol{x}) + \sin(u(\boldsymbol{x})) = g(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{B}^d = \{\boldsymbol{x} \mid \|\boldsymbol{x}\|_2 < 1\}, \tag{19}$$

$$u(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \mathbb{S}^{d-1} = \{\boldsymbol{x} \mid \|\boldsymbol{x}\|_2 = 1\}, \tag{20}$$

where $g(\boldsymbol{x}) = \Delta u_{\text{exact}}(\boldsymbol{x}) + \sin(u_{\text{exact}}(\boldsymbol{x}))$, since its nonlinearity order is infinity, i.e., its nonlinearity is strong.

Here are the implementation details. The model is a 4-layer fully connected network with 128 hidden units, which is trained via Adam [37] for 10K epochs in the two-body case and 20K epochs in the three-body case, respectively, with an initial learning rate 1e-3, which linearly decays to zero at the end of the optimization. We select 100 random residual points at each Adam epoch and 20K fixed testing points uniformly from the unit ball. We adopt the following model structure to satisfy the zero boundary condition with hard constraint and to avoid the boundary loss [38] $(1 - \|\boldsymbol{x}\|_2^2)u_\theta(\boldsymbol{x})$, where $u_\theta(\boldsymbol{x})$ is the neural neural network model. We repeat our experiment five times with five independent random seeds and report the mean and standard deviation of the errors. For HTE, we choose $V = 16$. For SDGD, we chose the batch size of dimension 16.

Method	Metric	100 D	1,000 D	5,000D	10,000 D	100,000 D
PINNs [45]	Speed	1367.61it/s	141.45it/s	8.43it/s	N.A.	N.A.
	Memory	1123MB	2915MB	14283MB	>80GB	>80GB
	Error_1	6.24E-3±2.83E-3	1.20E-3±6.47E-4	2.64E-3±1.33E-3	N.A.	N.A.
	Error_2	7.43E-3±4.56E-4	1.00E-3±1.45E-5	2.02E-4±2.45E-6	N.A.	N.A.
SDGD [22]	Speed	1853.67it/s	1444.00it/s	1243.91it/s	1027.38it/s	356.62it/s
	Memory	883MB	885MB	909MB	929MB	1173MB
	Error_1	6.28E-3±2.55E-3	1.55E-03±6.72E-4	2.63E-3±1.21E-3	1.93E-3±7.81E-4	2.30E-3±1.33E-3
	Error_2	7.60E-3±6.00E-4	1.15E-3±2.80E-4	2.05E-4±3.98E-6	1.04E-4±4.30E-6	1.56E-5±9.57E-6
HTE (Ours)	Speed	1792.03it/s	1566.19it/s	1275.81it/s	1066.10it/s	345.10it/s
	Memory	869MB	890MB	913MB	927MB	1089MB
	Error_1	6.30E-3±2.88E-3	1.25E-3±3.40E-4	2.61E-3±1.31E-3	1.84E-3±9.56E-4	2.38E-3±1.72E-3
	Error_2	7.58E-3±5.39E-4	9.94E-4±3.23E-6	2.01E-4±2.27E-6	1.02E-4±3.88E-6	1.59E-5±9.29E-6

Table 1: Computational results for Sine-Gordon equations with the two-body (Error_1) and three-body (Error_2) exact solutions.

The computational results for the two-body and three-body cases are presented in Table 1, where we compare vanilla PINN [45], SDGD [22], and HTE (Ours), in terms of speed (iteration per second), memory cost, and relative L_2 error for the two-body case (Error_1) and that for the three body case (Error_2). Note that when solving for the two PDEs with different solutions, the speed and the memory costs are similar, and only the error differs, so we only report speed and memory once.

Regarding the regular PINNs, we observe a significant slowdown in speed and a rapid increase in memory consumption as the dimensionality rises. This is because the regular PINNs require the computation of the full Hessian, and the computational cost quadratically increases with dimension. As a result, regular PINNs exceed the memory limit of an A100 GPU in the case of 10K dimensions. For HTE and SDGD, we observe similar convergence speeds, results and memory consumption. In scenarios with 100D, 1K D, and 5K D, the final errors are comparable to regular PINNs, demonstrating that HTE can overcome the curse-of-dimensionality. It accelerates regular PINNs without compromising its effectiveness. Moreover, the PDEs we used cannot be simplified into lower-dimensional subproblems as they are inherently high-dimensional. We also conducted tests on the PDE exact solutions of two-body and three-body interactions to demonstrate the efficacy of HTE across various high-dimensional problems.

4.2 High-Dimensional Gradient-Enhanced PINN

The Gradient-Enhanced Physics-Informed Neural Network (gPINN) [55] is a technique designed to enhance the performance of PINNs. It achieves this by incorporating additional regularization through the computation of an extra first-order derivative for the PINN's residual loss. However, due to the extra derivatives, gPINN becomes computationally expensive, particularly in higher dimensions, where the required additional derivatives are proportional to the dimensionality of the PDE. In this subsection, we illustrate how to leverage the proposed HTE method to expedite the training of gPINN. To illustrate, we continue to consider the Sine-Gordon equation with a two-body interactive solution discussed in the preceding section in equation (17).

Given the Sine-Gordon equation

$$\Delta u(\boldsymbol{x}) + \sin(u(\boldsymbol{x})) = g(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{B}^d = \{\boldsymbol{x} \mid \|\boldsymbol{x}\|_2 < 1\}, \tag{21}$$

$$u(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \mathbb{S}^{d-1} = \{\boldsymbol{x} \mid \|\boldsymbol{x}\|_2 = 1\}, \tag{22}$$

where $g(\boldsymbol{x}) = \Delta u_{\text{exact}}(\boldsymbol{x}) + \sin(u_{\text{exact}}(\boldsymbol{x}))$, the PINN loss is given by

$$L_{\text{PINN}}(\theta) = \frac{1}{2}\left(u_\theta(\boldsymbol{x}) + \sin(u_\theta(\boldsymbol{x})) - g(\boldsymbol{x})\right)^2 := \frac{1}{2}r_\theta(\boldsymbol{x})^2, \tag{23}$$

where $r_\theta(\boldsymbol{x}) = \Delta u_\theta(\boldsymbol{x}) + \sin(u_\theta(\boldsymbol{x})) - g(\boldsymbol{x})$ is the residual prediction. The gPINN loss is given by

$$L_{\text{gPINN}}(\theta) = \frac{1}{2} r_\theta(\boldsymbol{x})^2 + \frac{1}{2}\lambda_{\text{gPINN}} \|\nabla_{\boldsymbol{x}} r_\theta(\boldsymbol{x})\|^2, \tag{24}$$

i.e., gPINN optimizes both the residual part and its derivative to be zero, where $\lambda_{\text{gPINN}} \in \mathbb{R}^+$ is the weight for the gPINN regularization. To accelerate gPINN, we use the HTE-based gPINN loss

$$L_{\text{HTE, gPINN}}(\theta) = \frac{1}{2}\hat{r}_\theta(\boldsymbol{x})^2 + \frac{1}{2}\lambda_{\text{gPINN}} \|\nabla_{\boldsymbol{x}} \hat{r}_\theta(\boldsymbol{x})\|^2, \tag{25}$$

where $\hat{r}_\theta(\boldsymbol{x}) = \frac{1}{V}\sum_{i=1}^{V} \boldsymbol{v}_i^{\mathrm{T}} \left(\text{Hess } u_\theta(\boldsymbol{x})\right) \boldsymbol{v}_i + \sin(u_\theta(\boldsymbol{x})) - g(\boldsymbol{x})$ is the HTE-based residual prediction. Thus, we are only required to take an additional derivative to the HVP of the neural network model, which is much more efficient than that of the full Hessian.

The implementation details are given as follows. The model is a 4-layer fully connected network with 128 hidden units, which is trained via Adam [37] for 10K epochs with an initial learning rate 1e-3, which linearly decays to zero at the end of the optimization. We select 100 random residual points at each Adam epoch and 20K fixed testing points uniformly from the unit ball. We adopt the following model structure to satisfy the zero boundary condition with hard constraint and to avoid the boundary loss [38] $(1 - \|\boldsymbol{x}\|_2^2)u_\theta(\boldsymbol{x})$, where $u_\theta(\boldsymbol{x})$ is the neural neural network model. We repeat our experiment five times with five independent random seeds and report the mean and standard deviation of the errors. For HTE, we choose $V = 16$ in all settings. We choose λ_{gPINN} as ten in 100D and 1K D cases and choose it as ten thousand in 10K D and 100K D cases. The gPINN loss weight λ_{gPINN} can be chosen to make the scale of the PINN loss and the scale of the gPINN loss similar during initialization, i.e., choose λ_{gPINN} such that $r_\theta(\boldsymbol{x})^2 \approx \lambda_{\text{gPINN}} \|\nabla_{\boldsymbol{x}} r_\theta(\boldsymbol{x})\|^2$ and $\hat{r}_\theta(\boldsymbol{x})^2 \approx \lambda_{\text{gPINN}} \|\nabla_{\boldsymbol{x}} \hat{r}_\theta(\boldsymbol{x})\|^2$ at initialization.

Method	Metric	100D	1K D	10K D	100K D
PINN [45]	Speed	1367.61it/s	141.45it/s	N.A.	N.A.
	Error	6.24E-3±2.83E-3	1.20E-3±6.47E-4	N.A.	N.A.
gPINN [55]	Speed	458.84it/s	51.42it/s	N.A.	N.A.
	Error	4.20E-3±1.21E-2	4.42E-4±1.84E-4	N.A.	N.A.
HTE PINN (Ours)	Speed	1792.03it/s	1566.19it/s	1066.10it/s	345.10it/s
	Error	6.30E-3±2.88E-3	1.25E-3±3.40E-4	1.84E-3±9.56E-4	2.38E-3±1.72E-3
HTE gPINN (Ours)	Speed	616.79it/s	461.81it/s	229.18it/s	153.35it/s
	Error	5.08E-3±2.00E-3	4.88E-4±1.59E-4	4.68E-4±4.61E-4	4.77E-5±4.70E-5

Table 2: Computation results for gPINN.

The computational results are presented in Table 2, where three algorithms are compared: vanilla PINN [45], vanilla gPINN [55], HTE-based PINN, and HTE-based gPINN. In the preliminary, we observe that both PINN and gPINN encounter failure when exceeding the 80GB memory limit of the A100 GPU in dimensions surpassing 1000D. Conversely, PINN and gPINN based on HTE successfully operate in dimensions as high as 100K, demonstrating swift performance. Comparing PINN and gPINN, we note an enhancement in the latter's performance improvement, albeit at a slightly slower convergence pace, due to the additional first-order derivatives of the residual. The advantages of gPINN become more pronounced in higher dimensions (exceeding 1000D), leading to an additional order of magnitude reduction in PINN error. However, in scenarios with 100D and 1000D, HTE-based gPINN performs slightly inferior to conventional gPINN. This arises because HTE is ultimately an approximation, and in high-dimensional gPINN, it introduces d additional losses, where d is the dimensionality. Hence, the approximation with HTE tends to incur more significant errors. Nevertheless, the performance of HTE-based gPINN remains comparable to conventional gPINN. In summary, we verify that HTE can accelerate and scale up gPINN to very high dimensions. Moreover, gPINN continues to enhance the performance of PINN in high-dimensional PDEs. To the best of our knowledge, previous work [55] only demonstrated gPINN's effectiveness in low-dimensional PDEs, while our work is the first to show that in high dimensions.

4.3 Biharmonic Equation

In this subsection, we further validate the proposed HTE method, demonstrating its capability to accelerate the convergence of PINNs in high-dimensional and high-order biharmonic equations while significantly reducing its memory consumption. The following complicated exact solution is considered to test the convergence of high-

dimensional PDE solvers:

$$u_{\text{exact}}(\boldsymbol{x}) = \left(1 - \|\boldsymbol{x}\|_2^2\right)\left(4 - \|\boldsymbol{x}\|_2^2\right)\left(\sum_{i=1}^{d-2} c_i \exp(\boldsymbol{x}_i \boldsymbol{x}_{i+1} \boldsymbol{x}_{i+2})\right), \tag{26}$$

where $c_i \sim \mathcal{N}(0,1)$. The term $(1 - \|\boldsymbol{x}\|_2^2)(4 - \|\boldsymbol{x}\|_2^2)$ is multiplied for zero boundary condition to prevent the boundary loss from leaking the solution's information.

The Biharmonic equation is given as below

$$\Delta^2 u(\boldsymbol{x}) = g(\boldsymbol{x}), \quad \boldsymbol{x} \in \{\boldsymbol{x} \mid 1 < \|\boldsymbol{x}\|_2 < 2\}, \tag{27}$$

$$u(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \{\boldsymbol{x} \mid \|\boldsymbol{x}\|_2 = 1\} \cup \{\boldsymbol{x} \mid \|\boldsymbol{x}\|_2 = 2\}, \tag{28}$$

where $g(\boldsymbol{x}) = \Delta^2 u_{\text{exact}}(\boldsymbol{x})$ is given by the exact solution.

Here are the implementation details. The model is a 4-layer fully connected network with 128 hidden units, which is trained via Adam [37] for 10K epochs in 100D, 150D, and 200D cases, and 20K epochs in the 50D case, with an initial learning rate 1e-3, which linearly decays to zero at the end of the optimization. We select 100 random residual points at each Adam epoch and 20K fixed testing points within the domain $\boldsymbol{x} \in \{\boldsymbol{x} \mid 1 \le \|\boldsymbol{x}\|_2 \le 2\}$. We adopt the following model structure to satisfy the zero boundary condition with hard constraint and to avoid the boundary loss [38]: $(1 - \|\boldsymbol{x}\|_2^2)(4 - \|\boldsymbol{x}\|_2^2)u_\theta(\boldsymbol{x})$, where $u_\theta(\boldsymbol{x})$ is the neural neural network model. We repeat our experiment five times with five independent random seeds and report the mean and standard deviation of the errors. For HTE, we control the batch size $V = 16/512/1024$ to see how V affects convergence.

Method	Metric	50D	100D	150D	200D
PINN [45]	Speed	19.82it/s	6.56it/s	3.50it/s	N.A.
	Memory	6199MB	21453MB	44631MB	>80GB
	Error	2.34E-2±1.91E-2	6.01E-3±2.32E-3	3.11E-3±1.79E-3	N.A.
HTE ($V = 16$)	Speed	438.79it/s	109.57it/s	54.86it/s	25.89it/s
	Memory	991MB	2085MB	3589MB	7225MB
	Error	2.36E-2±1.97E-2	6.83E-3±1.63E-3	3.91E-3±1.47E-3	4.40E-3±5.65E-3
HTE ($V = 512$)	Speed	123.98it/s	54.07it/s	42.44it/s	23.50it/s
	Memory	1861MB	2089MB	3593MB	7229MB
	Error	2.34E-2±1.96E-2	6.08E-3±2.28E-3	3.39E-3±1.99E-3	4.03E-3±4.85E-3
HTE ($V = 1024$)	Speed	78.50it/s	34.72it/s	33.77it/s	20.36it/s
	Memory	2535MB	3037MB	3595MB	7231MB
	Error	2.34E-2±1.96E-2	6.01E-3±2.35E-3	3.13E-3±1.82E-3	3.97E-3±4.91E-3

Table 3: Computational results for the Biharmonic equation.

The computational results for the biharmonic equation are presented in Table 3, where we report the speed, memory, and relative L_2 error of the baseline PINN and our proposed HTE method. Regarding the regular PINN, we observe a significant slowdown in speed and a rapid increase in memory consumption as the dimensionality rises. This is because the regular PINNs require the computation of the full biharmonic operator, and the computational cost increases to the fourth power with respect to the dimension. As a result, regular PINNs exceed the memory limit of an A100 GPU in the case of 200 dimensions. In contrast, the second-order PDE case requires 10K dimensions for PINN to go out-of-memory, signifying that the biharmonic operator is much more costly than the Hessian due to the high-order derivative. For HTE, we opted for a batch size of $V = 512/1024$ to make HTE's convergence results similar to those of PINN, which is in contrast to our earlier example with a second-order PDE, where we used a batch size of $V = 16$. If we just use a small batch size $V = 16$ in the biharmonic equation, then HTE will perform worse than PINN. The reason behind this is our variance analysis, indicating that when estimating the biharmonic operator, both diagonal and off-diagonal elements contribute to the variance, resulting in relatively larger errors than estimating the Hessian trace. Nevertheless, HTE demonstrates substantial improvements in terms of speed and memory consumption. In scenarios exceeding 50 dimensions, its speed is nearly ten times that of regular PINN, and the rate of memory consumption growth is significantly lower than that of PINN.

5 Summary

In this paper, we introduced the Hutchinson Trace Estimation (HTE) method to enhance the range of capabilities of Physics-Informed Neural Networks (PINNs) in tackling high-dimensional and high-order partial differential equations

(PDEs). While PINNs have succeeded in low-dimensional problems, their application to complex PDEs has faced challenges due to computational bottlenecks in automatic differentiation. HTE, which is applied to calculate Hessian vector products (HVPs), has emerged as an effective solution to accelerate PINNs and reduce memory costs.

We first validated our approach on second-order parabolic equations, demonstrating the convergence of the PINN loss with HTE to the original PINNs loss under certain conditions, guaranteeing the effectiveness of the HTE approximation. Comparisons with Stochastic Dimension Gradient Descent (SDGD) highlighted the superior performance of HTE in scenarios with significant dimensionality variability and variance, where we delved into the theoretical comparison between the two methods by proving their corresponding variance. The extension of HTE to the biharmonic equation showcased its efficiency in handling higher-order, high-dimensional PDEs by employing tensor-vector products (TVPs) to transform computations.

Experimental setups confirmed the effectiveness of HTE, revealing comparable convergence effects with SDGD under memory and speed constraints. Furthermore, HTE proved valuable in accelerating Gradient-Enhanced PINN (gPINN), which requires an additional first-order derivative over the PINNs residual and the fourth-order high dimensional biharmonic equation for better computational efficiency.

In conclusion, our proposed HTE method addresses the limitations of PINNs in handling high-dimensional and high-order PDEs, providing a versatile and efficient approach. Our work contributes to the scientific machine learning field by presenting a unified framework for solving general high-dimensional PDEs, demonstrating the effectiveness of HTE, and discussing its advantages over existing methods.

Acknowledgement

A Proof

A.1 Proof of Theorem 3.1

Convergence of $L_{\textbf{HTE}}(\theta; \{\boldsymbol{v}_i\}_{i=1}^V)$. Due to the strong law of large numbers,

$$\mathbb{P}\left(\lim_{V\to\infty} \frac{1}{V}\sum_{i=1}^V \boldsymbol{v}_i^{\mathrm{T}} A_\theta(\boldsymbol{x},t)\boldsymbol{v}_i = \mathrm{Tr}\left(A_\theta(\boldsymbol{x},t)\right)\right) = 1. \tag{29}$$

Thus,

$$\mathbb{P}\left(\lim_{V\to\infty}\left(\frac{1}{V}\sum_{i=1}^V \boldsymbol{v}_i^{\mathrm{T}} A_\theta(\boldsymbol{x},t)\boldsymbol{v}_i + B_\theta(\boldsymbol{x},t)\right)^2 = \left(\mathrm{Tr}\left(A_\theta(\boldsymbol{x},t)\right) + B_\theta(\boldsymbol{x},t)\right)^2\right) = 1. \tag{30}$$

Unbiasedness of $L_{\textbf{HTE, unbiased}}(\theta; \{\boldsymbol{v}_i, \hat{\boldsymbol{v}}_i\}_{i=1}^V)$. Since HTE is an unbiased trace estimator,

$$\begin{aligned}
&\mathbb{E}_{\{\boldsymbol{v}_i,\hat{\boldsymbol{v}}_i\}_{i=1}^V}\left[L_{\text{HTE, unbiased}}(\theta; \{\boldsymbol{v}_i,\hat{\boldsymbol{v}}_i\}_{i=1}^V)\right]\\
&= \frac{1}{2}\mathbb{E}_{\{\boldsymbol{v}_i\}_{i=1}^V}\left[\frac{1}{V}\sum_{i=1}^V \boldsymbol{v}_i^{\mathrm{T}} A_\theta(\boldsymbol{x},t)\boldsymbol{v}_i + B_\theta(\boldsymbol{x},t)\right]\mathbb{E}_{\{\hat{\boldsymbol{v}}_i\}_{i=1}^V}\left[\frac{1}{V}\sum_{i=1}^V \hat{\boldsymbol{v}}_i^{\mathrm{T}} A_\theta(\boldsymbol{x},t)\hat{\boldsymbol{v}}_i + B_\theta(\boldsymbol{x},t)\right]\\
&= \frac{1}{2}\left[\mathrm{Tr}\left(A_\theta(\boldsymbol{x},t)\right) + B_\theta(\boldsymbol{x},t)\right]^2\\
&= L_{\text{PINN}}(\theta).
\end{aligned} \tag{31}$$

A.2 Proof of Theorem 3.4

For the unit Gaussian distribution, we have that

$$\begin{aligned}
\mathbb{E}_{\boldsymbol{v}\sim\mathcal{N}(0,I)}\left[\frac{\partial^4}{\partial\boldsymbol{x}^4}u(\boldsymbol{x})[\boldsymbol{v},\boldsymbol{v},\boldsymbol{v},\boldsymbol{v}]\right] &= \mathbb{E}_{\boldsymbol{v}\sim\mathcal{N}(0,I)}\left[\sum_{i,j,k,l=1}^d \frac{\partial^4}{\partial\boldsymbol{x}_i\partial\boldsymbol{x}_j\partial\boldsymbol{x}_k\partial\boldsymbol{x}_l}u(\boldsymbol{x})\boldsymbol{v}_i\boldsymbol{v}_j\boldsymbol{v}_k\boldsymbol{v}_l\right]\\
&= \mathbb{E}_{\boldsymbol{v}\sim\mathcal{N}(0,I)}\left[\sum_{i=1}^d \frac{\partial^4}{\partial\boldsymbol{x}_i^4}u(\boldsymbol{x})\boldsymbol{v}_i^4\right] + 6\mathbb{E}_{\boldsymbol{v}\sim\mathcal{N}(0,I)}\left[\sum_{i\neq j}\frac{\partial^4}{\partial\boldsymbol{x}_i^2\partial\boldsymbol{x}_j^2}u(\boldsymbol{x})\boldsymbol{v}_i^2\boldsymbol{v}_j^2\right]\\
&= 3\sum_{i=1}^d \frac{\partial^4}{\partial\boldsymbol{x}_i^4}u(\boldsymbol{x}) + 6\sum_{i\neq j}\frac{\partial^4}{\partial\boldsymbol{x}_i^2\partial\boldsymbol{x}_j^2}u(\boldsymbol{x})\\
&= 3\Delta^2 u(\boldsymbol{x}).
\end{aligned} \tag{32}$$

A.3 Proof of Theorem 3.2

SDGD's trace estimator is $\mathrm{Tr}(A) \approx \frac{d}{|I|}\sum_{i\in I} A_{ii}$. Suppose that the batch size of the sampled dimension in SDGD is B; then the variance can be directly computed:

$$\mathbb{V}\left[\frac{d}{B}\sum_{i\in I} A_{ii}\right] = \frac{1}{\binom{d}{B}}\left(\sum_{I:|I|=B}\frac{d}{B}\sum_{i\in I} A_{ii} - \sum_{i=1}^d A_{ii}\right)^2, \tag{33}$$

where $\binom{d}{B} = \frac{d(d-1)\cdots(d-B+1)}{B(B-1)\cdots 1}$.

A.4 Proof of Theorem 3.3

The estimator of HTE is $\mathrm{Tr}(A) \approx \frac{1}{V}\sum_{k=1}^V \boldsymbol{v}_k^{\mathrm{T}} A\boldsymbol{v}_k = \sum_{i=1}^d A_{ii} + \frac{1}{V}\sum_{i\neq j} A_{ij}\sum_{k=1}^V \boldsymbol{v}_{k,i}\boldsymbol{v}_{k,j}$, where $\boldsymbol{v}_{k,i}$ denotes the ith dimension of the vector $\boldsymbol{v}_k \in \mathbb{R}^d$ and we are using $p(\boldsymbol{v})$ as the Rademacher distribution.

HTE's variance can be computed as follows:

$$\begin{aligned}
\left(\boldsymbol{v}^{\mathrm{T}} A\boldsymbol{v} - \mathrm{Tr}(A)\right)^2 &= \left(\sum_{i\neq j} A_{ij}\boldsymbol{v}_i\boldsymbol{v}_j\right)^2\\
&= \sum_{i\neq j}\sum_{k\neq l} A_{ij}A_{kl}\boldsymbol{v}_i\boldsymbol{v}_j\boldsymbol{v}_k\boldsymbol{v}_l.
\end{aligned} \tag{34}$$

If $i = k$ and $j = l$, then $\mathbb{E}[\boldsymbol{v}_i \boldsymbol{v}_j \boldsymbol{v}_k \boldsymbol{v}_l] = \mathbb{E}[v_i^2]\mathbb{E}[v_j^2] = 1$, else equals zero. Therefore,

$$\mathbb{V}\left[\boldsymbol{v}^{\mathrm{T}} A \boldsymbol{v}\right] = \mathbb{E}\left[\left(\boldsymbol{v}^{\mathrm{T}} A \boldsymbol{v} - \mathrm{Tr}(A)\right)^2\right] = \sum_{i \neq j} A_{ij}^2. \tag{35}$$

With the HTE estimator of batch size V, the variance is

$$\mathbb{V}\left[\frac{1}{V}\sum_{k=1}^{V} \boldsymbol{v}_k^{\mathrm{T}} A \boldsymbol{v}_k\right] = \frac{1}{V}\sum_{i \neq j} A_{ij}^2. \tag{36}$$

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