PHYSICS-INFORMED NEURAL NETWORKS FOR OPERATOR EQUATIONS
WITH STOCHASTIC DATA

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Abstract. We consider the computation of statistical moments to operator equations with stochastic data. We remark that application of PINNs—referred to as TPINNs—allows to solve the induced tensor operator equations under minimal changes of existing PINNs code, and enabling handling of non-linear and time-dependent operators. We propose two types of architectures, referred to as vanilla and multi-output TPINNs, and investigate their benefits and limitations. Exhaustive numerical experiments are performed; demonstrating applicability and performance; raising a variety of new promising research avenues.

Key words. physics-informed neural networks, uncertainty quantification, tensor operator equations

MSC codes. 65Mxx, 35R60

1. Introduction. Uncertainty quantification (UQ) is paramount in domains ranging from aerospace exploration to electronic design automation. Uncertain data or source term delivers an abstract operator equation with stochastic data of the form:

\[ A u(\omega) = f(\omega) \quad \mathbb{P}\text{-a.e. } \omega \in \Omega. \]  

We aim at computing the statistical moments for \( u(\omega) \), as being for any integer \( k \geq 1 \):

\[ \mathcal{M}_k[u] := \int \Omega u(x_1, \omega) \cdots u(x_k, \omega) d\mathbb{P}, \]

the latter amounting to solving the following tensor operator equation:

\[ (A \otimes \cdots \otimes A) \mathcal{M}_k[u] = \mathcal{M}_k[f]. \]

Tensor operator equations are prone to the infamous curse of dimensionality [32]. To circumvent this limitation, coupling: (i) numerical scheme such as finite or boundary element methods [30]; with (ii) sparse tensor approximation [12] is common in literature. We refer to the reference work of von Petersdorff and Schwab [32] and applications [14, 9, 11].

However, the aforementioned method:
1. Restricts to strongly elliptic linear operators [32, Section 2];
2. Can be non-trivial to implement, as numerical solvers are not adapted to high-order tensors. Indeed, they commonly only deliver matrix-product operations;
3. Leads to optimal yet possibly slow convergence for iterative solvers [9, Section 6.2].

Concerning Item 1., non-linear operators are amenable to linear tensor equations with stochastic data under additional requirements [7]. Regarding Item 2., notice that for matrices \( A, X \in \mathbb{C}^{N,N} \) and integer \( N \geq 1 \), there holds that [20]:

\[ (A \otimes \cdots \otimes A) \text{vec}(X) = AXA^T, \]

where \( \text{vec}(X) \) stacks the columns of \( X \) one below the others, and \( A^T \) is the transpose of \( A \). This allows to solve tensor operator equations for \( k = 2 \) provided a matrix-matrix class. We refer the reader to [20, Section 2.2] for higher \( k \) and sparse matrices. To the authors’ knowledge, numerical experiments in the literature are restricted to \( k = 2 \), despite enjoying a complete theory [28].

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Recently, physics-informed neural networks (PINNs) were introduced in [26]. Praised for their versatility, they apply to forward and inverse problems involving partial differential equations (PDEs). They are constructed over deep neural networks [3], inheriting their capability to approximate high-dimensional and non-linear mappings [29, 27]. Amongst other applications of PINNs, we mention inverse problems [6], inverse design [19], and fractional operators [24]. Recently, Mishra and Molinaro [22, 21] proposed a general theory to quantify the generalization error for PINNs.

All throughout, we restrict to UQ for deterministic PDEs with a random load in (1.1). For the sake of completeness, we mention UQ for parametric stochastic operators [8] (e.g. elliptic operators [2]) and for stochastic PDEs via PINNs [37]. Furthermore, deep neural networks (resp. PINNs) were used to model uncertain surrogates [27, 31] (resp. [40]). We also put forth Bayesian PINNs [34], PINNs for determining the total uncertainty [38], and GAN PINNs [36]. A complete overview of these methods and their practical implementation is available in NeuralUQ [41]. Lastly, we mention multi-output (MO)-PINNs for UQ [35].

In this work, we apply PINNs to tensor operator equations, referred to as Tensor PINNs (TPINNs). These novel PINNs inherits the following interesting properties:

✓ They scale well with increasing k;
✓ They require minimal changes—specifically, adapt the data generation—to existing PINNs code;
✓ They allow to consider time-dependent and non-linear problems;
✓ They can be extended to—ill-posed—inverse problems [6].

Moreover, PINNs solve operator equations in strong form. This allows for a rather simple expression for the Kronecker product (as opposed to operators equations in weak form [32] or matrices). Furthermore, operator equations can often be described in (higher) mixed Sobolev regularity spaces [32], this extra natural smoothness supporting the use of strong form—though being out of the scope of this work.

Inspired by the framework in [22], we provide a bound for the generalization error of vanilla (V)-TPINNs in Theorem 4.1. This result allows to understand better TPINNs and supplies a strong theoretical background to their formulation.

Alongside, we remark that TPINNs involve higher order differentiation as k increases (refer also to [39, 13]). Accordingly, we introduce a MO variant of V-TPINNs, referred to as MO-TPINNs, and applicable for the scalar case. It consists of using successive applications of the operator as variables, bounding the order of differentiation for the loss with k. This results in lowering the computational cost at the expense of an increase of hyper-parameters—the k terms in the loss function.

Numerical experiments demonstrate the practical simplicity of TPINNs and their prominent performance. They allow to obtain a surprisingly accurate approximation for few collocation points $N$ and training epochs, e.g. a $L^2$ relative error of $\sim 5\%$ for $N \sim 10^3$ collocation points after $\sim 10^4$ epochs for $k = 2$ and a two dimensional Helmholtz equation (see later on in Subsection 6.4).

We provide a fair comparison of V-TPINNs and MO-TPINNs, and study the trade-off between training performance and computational requirements. We consider separable and Gaussian co-variance kernels as right-hand side. This work is structured as follows: We formulate the framework for operator equations with stochastic data in Section 2, we introduce TPINNs in Section 3 and supply convergence analysis in Section 4. Next, we discuss implementation in Section 5, we present numerical experiments in Section 6 and conclude in Section 7.

2. Operator equations with stochastic data. To begin with, we set the notations that will be used all throughout this manuscript.

2.1. General Notation. For a natural number k, we set $\mathbb{N}_k := \{k, k + 1, \cdots \}$. Let $D \subseteq \mathbb{R}^d$ for $d \in \mathbb{N}_1$ be an open set. For $p > 0$, $L^p(D)$ is the standard class of functions with bounded $L^p$-norm over $D$. Given $s \in \mathbb{R}$, $q \geq 0$, $p \in [1, \infty]$, we refer to [30] for the definitions of Sobolev function spaces $H^s(D)$. Norms are denoted by $\| \cdot \|$ with subscripts indicating the associated

1https://github.com/Crunch-UQ4MI/neuraluq
functional space. For $k \in \mathbb{N}_1$ and $x_i \in \mathbb{R}^d$, $i = 1, \ldots, k$, we set $x := (x_1, \ldots, x_k)$. $k$-fold tensors quantities are denoted with parenthesized superscripts, e.g. $f^{(k)} := f \otimes \cdots \otimes f$. Their diagonal part is referred as:

\begin{equation}
\text{diag}(f^{(k)}) = f^{(k)}|_{x_1=\ldots=x_k} = f(x_1) \otimes \cdots \otimes f(x_1).
\end{equation}

For $X, Y$ separable Hilbert spaces, we set $A \in \mathcal{B}(X, Y)$ the space of bounded mappings from $X$ to $Y$ and define the unique bounded tensor product operator [23]:

\begin{equation}
A^{(k)} := A \otimes \cdots \otimes A \in \mathcal{B}(X^{(k)}, Y^{(k)}).
\end{equation}

Notice that if $A$ is continuous, $\mathcal{B}(X, Y) \equiv \mathcal{L}(X, Y)$, the latter being the space of continuous linear operators.

2.2. Abstract problem. All throughout this manuscript, let $(\Omega, \mathcal{A}, P)$ be a probability space, $X, Y$ separable Hilbert spaces, and $k \in \mathbb{N}_1$. For $u : \Omega \to X$ a random field in the Bochner space $L^k(\Omega, \mathcal{A}, P)$ [32], we introduce the statistical moments:

\begin{equation}
\mathcal{M}^k[u(\omega)] := \int_{\Omega} u(x_1, \omega) \cdots u(x_k, \omega) dP(\omega),
\end{equation}

with $\mathcal{M}^1 = \mathbb{E}$ being the expectation.

The abstract problem reads: Given $A : X \to Y$ and $f \in L^k(\Omega, \mathcal{A}, P; Y)$, we seek $u \in L^k(\Omega, \mathcal{A}, P; X)$ such that:

\begin{equation}
Au(\omega) = b(\omega) \quad \text{for } P\text{-a.e. } \omega \in \Omega.
\end{equation}

Application of (2.2) to (2.3) yields the following operator equation: Given $C^k := \mathcal{M}^k[f] \in Y^{(k)}$, we seek $\Sigma^k := \mathcal{M}^k[u] \in X^{(k)}$ such that:

\begin{equation}
A^{(k)}\Sigma^k = C^k.
\end{equation}

In the sequel, we assume that (2.4) has a unique solution. Furthermore, we suppose that $A$ admits a linearization $L \in \mathcal{L}(X, Y)$ with bounded inverse $L^{-1} \in \mathcal{L}(Y, X)$, i.e.

\begin{equation}
Au - Av = L(u - v) \quad \forall u, v \in X
\end{equation}

with

\begin{equation}
\|L^{-1}\|_{Y \to X} \leq \gamma_L^{-1} < \infty
\end{equation}

wherein $\gamma_L > 0$. This setting corresponds to Example 2 in [22, Section 2.1]. Thus, one has that for any $u, v \in X$:

\begin{equation}
\|u - v\|_X = \|L^{-1}(Au - Av)\|_X \leq \gamma_L^{-1}\|Au - Av\|_Y.
\end{equation}

As a consequence, application of the statistical moments to (2.5) for $u, v \in L^k(\Omega, \mathcal{A}, P; X)$ yields a linearization for $A^{(k)}$ as:

\begin{equation}
A^{(k)}U - A^{(k)}V = L^{(k)}(U - V),
\end{equation}

wherein $U := \mathcal{M}^{(k)}[u]$ and $V := \mathcal{M}^{(k)}[v]$. Finally, there holds that:

\begin{equation}
\|U - V\|_{X^{(k)}} = \left\|L^{-1}\right\|_{Y^{(k)}} \left\|A^{(k)}U - A^{(k)}V\right\|_{Y^{(k)}} \leq \frac{1}{\gamma_L^{k}} \left\|A^{(k)}U - A^{(k)}V\right\|_{Y^{(k)}}.
\end{equation}

Stability bound (2.7) will be key in yielding a bounded generalization error for TPINNs in Section 4.

Generally, operator equations are used to describe boundary value problems [32] and can be recast as:

\begin{equation}
A = (A_D, A_B)
\end{equation}

with $A_D$ and $A_B$ defined over vector spaces with values in $D$ and $\partial D$ respectively---$\partial D = \Gamma$ or $\Gamma \times (t = 0)$ for time-dependent problem. This observation will be key in simplifying TPINNs later on in Section 3.
3. TPINNs. The proposed method consists in solving operator equation (2.4) by means of PINNs. For the sake of simplicity, we restrict ourselves to $Y = L^2(D; \mathbb{R}^m)$. Notice that we could apply our framework to UQ for inverse problems (refer e.g. to [21]). Let $\sigma$ be a smooth activation function. Throughout, we consider an input $x = (x_1, \cdots, x_k) \in D^{(k)}$. Following [18, Section 2.1] and notations in [9], we define $\mathcal{N}^l$ as being a $L$-layer neural network with $N_l$ neurons in the $l$-th layer for $1 \leq l \leq L - 1$ ($N_0 = dk$ and $N_L$ to be determined later on). For $1 \leq l \leq L$, let us denote the weight matrix and bias vector in the $l$-th layer by $W^l \in \mathbb{R}^{N_{l-1} \times N_l}$ and $b^l \in \mathbb{R}^{N_l}$, respectively. A mapping $x \mapsto z(x)$ can be approximated by a deep (feedforward) neural network defined as follows:

$$z_1(x) = \sigma(W_1z_0(x) + b_1) \in \mathbb{R}^{N_1} \quad \text{for} \quad 1 \leq l \leq L - 1,$$

$$z_L(x) = \sigma(W_Lz_{L-1}(x) + b_L) \in \mathbb{R}^{N_L}.$$

Finally, we introduce the collocation points $T := \{ x_i \mid x_i \in D^{(k)} \}_{i=1}^N$ of cardinality $N \in \mathbb{N}_1$. PINNs are commonly optimized via ADAM [15] with a given learning rate $\ell$, over a fixed number of epochs. Derivatives are evaluated by means of automatic differentiation (AD) [18], allowing us to consider general pseudo-differential operators. Further application of L-BFGS [17] can improve training [18].

In this work, we make an extensive use of hard boundary conditions (BCs) [19, 16, 18] in order to restrict the collocation points to $D^{(k)}$ and to greatly simplify TPINNs (refer to Remark 3.1 for more details). Hard BCs consist in applying a transformation $\Sigma^k \mapsto \tilde{\Sigma}^k$ in such a way that $\tilde{\Sigma}^k$ fulfills the BCs.

Remark 3.1 (Hard BCs). Using a transformation to enforce hard BCs allows to greatly simplify the formulation for TPINNs by reducing the tensor operator equation over $D^k$. For instance, let us consider the Laplace operator with Dirichlet BCs $\gamma_D u \mapsto u|\Gamma$. The formulation for $k = 2$ is

$$\begin{cases}
(-\Delta \otimes -\Delta) M^2[u] = M^2[f_D] \quad \text{in} \quad D \times D, \\
(-\Delta \otimes \gamma_D) M^2[u] = E[f_d g] \quad \text{in} \quad D \times \Gamma, \\
(\gamma_D \otimes -\Delta) M^2[u] = E[g f_D] \quad \text{in} \quad \Gamma \times D, \\
(\gamma_D \otimes \gamma_D) M^2[u] = M^2[g] \quad \text{on} \quad \Gamma \times \Gamma.
\end{cases}$$

In this case, the tensor equation for $k$ has $2^k$ terms, which would originate a $2^k$-terms loss function for V-TPINNs in (3.4).

One generally surveys that the model generalizes well by predicting the solution over a $N^{test}$-cardinality training set $T^{test}$ defined again over $D^{(k)}$. For TPINNs with constant width, we set $N = N_j$, $j = 1, \cdots, L - 1$.

3.1. V-TPINNs. V-TPINNs correspond to setting $N_L = m$ in (3.1) and applying (3.1) to (2.4), delivering an approximation

$$z^*_L = \Sigma^k_0.$$

The residual for V-TPINNs is:

$$\xi_\theta := A^{(k)} \Sigma^k_0 - C^k$$

and the loss function reads (for a MC points distribution):

$$\mathcal{L}_\theta := \frac{1}{N} \sum_{x \in T} \xi^2_\theta.$$

We seek at obtaining:

$$\theta^* := \text{argmin}_{\theta \in \Theta} \mathcal{L}_\theta.$$
with $\mathcal{L}_\theta$ in (3.4) yielding
\[(3.5)\]
$$\Sigma^k := \Sigma^{\theta}.$$ 

When hard BCs are used, notice that the residual (3.3) reduces to
\[
\xi^\theta := A^{(k)}\Sigma^k - C^k \text{ with } \Sigma^k \equiv \Sigma^{(k,\theta)} \text{ and } C_D = \mathcal{M}^k[f|D].
\]

An example of V-TPINN is showcased in Figure 3.1. It is paramount to note that the loss function has only one term, but that the latter involves the evaluation of $A^{(k)}$. Also, $k$ only impacts the input layer, affecting moderately—linearly—the size of the neural network.

3.2. MO-TPINNs. As will be noticed later in numerical experiments, V-TPINNs can become impractical for increasing $k$ when $A$ involves derivatives. For instance, set $A_D = -\Delta$ (refer e.g. to the example in Remark 3.1). The Laplace operator involves a second-order derivative; hence the TPINN loss involves $2k$-order derivatives. However, it is known that $AD$ scales poorly with high-order derivatives (refer to [39, 13]). To be precise, the computational requirements of $AD$ grow exponentially with the order of differentiation [4]. In [4], the authors propose a method to lower this cost for Jax [5] backend. Though, the latter does not allow to evaluate mixed derivatives, as occurs in V-TPINNs.

To remedy this concern, we introduce a MO architecture, inspired by local Galerkin methods [39] and [13].

Let us assume that $A = (A_D, A_B)$ in (2.8) and $N_L = m = 1$ in (3.1) i.e. $Y = L^2(D; \mathbb{R})$. There holds that:
\[
A_D \otimes \cdots \otimes A_D = A_D \circ \cdots \circ A_D.
\]

We set:
\[
(3.6) \begin{cases}
A_D V_1 &= C^k_D, \\
A_D V_2 &= V_1, \\
 \vdots &
\end{cases}
A_D \Sigma^k &= V_{k-1}.
\]

MO-TPINNs amount to use hard BCs and apply (3.1) to $(V_{1,\theta}, \cdots, V_{k,\theta})$ in (3.6), hence the approximate:
\[(3.7)\]
$$z^L = (V_{1,\theta}, \cdots, V_{k,\theta}).$$

Having introduced the residuals
\[(3.8)\]
$$\begin{cases}
\xi_1 &= A_D V_1 - C^k_D, \\
\xi_2 &= A_D V_2 - V_1, \\
 \vdots &
\end{cases}
\xi_k &= A_D \Sigma^k - V_{k-1},$$

Fig. 3.1: Schematic representation of a V-TPINN. The neural networks have $L - 1 = 2$ hidden layers.
the composite loss function is defined for any \( \omega_j > 0, j = 1, \cdots, k \) as:

\[
L_\theta = \sum_{j=1}^{k} \omega_j L^j_\theta
\]

with

\[
L^j_\theta = \frac{1}{N} \sum_{x \in T} \xi_{j, \theta}(x)^2.
\]

Acknowledge that the residual in (3.8) does not involve powers of \( A \), though inducing an output and loss function with \( k \) terms. In summary, we represent a MO-TPINN in Figure 3.2.

4. Convergence analysis for V-TPINNs. In this section, we apply the proceeding of [22] to V-TPINNs. We restrict to V-TPINNs, since stability bounds for MO-TPINNs are more involved and remain elusive. The residual PINNs loss in (3.4) induces approximating integrals for \( H \in Y^{(k)} = L^2(D; \mathbb{R}^m)^{(k)} \):

\[
\hat{H} = \int_{D^{(k)}} H(x_1, \cdots, x_k) \, dx_1 \cdots dx_k.
\]

We assume that we are given a quadrature to approximate \( \hat{H} \) as:

\[
\hat{H}_N := \sum_{i=1}^{N} w_i H(y^i)
\]

for weights \( w_i \) and quadrature points \( y^i \in D^{(k)} \). We further assume that the quadrature error is bounded as:

\[
|\hat{H}_N - \hat{H}| \leq c_{\text{quad}}(\|H\|_{Y^{(k)}}) N^{-\alpha}
\]

for some \( \alpha > 0 \). Concerning \( \alpha \), Monte-Carlo sampling methods yield \( \alpha = 1/2 \) in the root mean square and are a method of choice for very high dimensions [22]. Notice that we defined the loss in this sense in Equation (3.4) and (3.10). For moderately high dimensions, we can use Quasi Monte-Carlo sampling methods, whose performance relies on the smoothness of \( Y \).

We seek at quantifying the total error, also referred to as generalization error:

\[
\varepsilon_G = \varepsilon_G(\theta^*) := \| \Sigma^k_\theta - \Sigma^k_\theta \|_{X^{(k)}}
\]

with \( \Sigma^k_\theta \) and \( \Sigma^k_\theta \) in (3.2) and (3.5) respectively.

The training error is given by:

\[
\varepsilon_T(\theta)^2 = \sum_{i=1}^{N} w_i \xi_\star(y_i)^2 \approx \| \xi_\star \|_{Y^{(k)}}.
\]
Acknowledge that (4.3) measures the total error in the domain space, while (4.4) is for the residual in range space. We aim at understanding how these errors relate with each other.

In Figure 4.1, we depict the error for V-TPINNs. Remark that the generalization error is bounded from below by the best approximation error of the neural net class (the class of functions that the neural net can approximate).

\[
\sum_k \theta (N, \mathcal{NN}) \quad \sum_k \theta^* (N, \mathcal{NN}) \quad \sum_k (\mathcal{NN}) \quad \sum_k
\]

Neural net
optimization error
estimation error
approximation error
generalization error

Fig. 4.1: Illustration of the total error for TPINNs. In Theorem 4.1 we provide a bound for the generalization error for V-TPINNs.

We are ready to state a fundamental result of this work, namely a bound for the generalization error of V-TPINNs.

**Theorem 4.1 (Generalization error for V-TPINNs).** Under the present setting, the generalization error in (4.3) is bounded as:

\[
\varepsilon_G \leq \gamma_L^{-k} \varepsilon_T + \gamma_L^{-k} c_{\text{quad}} N^{-\alpha/2},
\]

with \( \gamma_L \) the stability constant in (2.6) and \( c_{\text{quad}} \) in (4.2).

**Proof.** Under the present setting, remark that:

\[
\varepsilon_T^2 = \| \Sigma^k - \Sigma^k \|_{X^{(k)}}^2 \quad \text{by definition (4.3)},
\]

\[
\leq \gamma_L^{-2k} \| A^{(k)} \Sigma^k - A^{(k)} \Sigma^k \|_{L^2(D)^{(k)}}^2 \quad \text{by application of (2.7) to } \Sigma^*, \Sigma^k = V,
\]

\[
= \gamma_L^{-2k} \| \xi^*_1 \|_{Y^{(k)}} \quad \text{by (3.3)},
\]

\[
\leq \gamma_L^{-2k} \left( \varepsilon_T^2 + c_{\text{quad}} N^{-\alpha} \right) \quad \text{by (4.2)},
\]

yielding the desired result.

Theorem 4.1 states that the generalization is bounded by: (i) one term depending on the training error (tractable) and (ii) another one depending on the number of collocation points. This shows that for enough collocation points, one has a controlled generalization error depending on the training error modulo the stability constant for the problem under consideration. Also, this result proves that the novel V-TPINNs has the same capabilities as PINNs, which will be verified in Section 6.

5. Implementation. We detail the implementation of TPINNs in DeepXDE [18]. Readers are referred to the preceding reference for the steps of general PINNs implementation. In Listing 1, we detail the code that was added to handle random sampling for tensor points \( x \in D^{(k)} \).

```python
1 class GeometryXGeometry:
2     def __init__(self, geometry, k):
3         self.geometry = geometry
4         self.dim = geometry.dim ** k
5         self.k = k
6
7     def random_points(self, n, random="pseudo"):
```

These few lines allow to sample random points in \( D^{(k)} \). Notice than one could handle soft BCs similarly by adding a method for random boundary points.
For the sake of clarity, we revisit the flowchart of PINNs according to DeepXDE [18, Figure 5] in Figure 5.1. We remark that TPINNs can be applied with minor changes to existing code (namely, the implementation of a sampler), and without having to access to the solver core. Specific loss and BCs are enforced via the main code.

Fig. 5.1: Flowchart of DeepXDE in [18, Figure 5] showing that TPINNs can be added to PINNs code with minor changes. The additions to the source code are in red. Boxes in green are adapted to the tensor setting in the main code via proper definition of the loss function and hard constraints.

6. Numerical experiments. In this section, we apply TPINNs to several operator equations.

6.1. Methodology. Throughout, we perform simulations with DeepXDE 1.7.1\textsuperscript{2} [18] in single float precision on a AMAX DL-E48A AMD Rome EPYC server with 8 Quadro RTX 8000 Nvidia GPUs—each one with a 48 GB memory. We use TensorFlow 2.5.0 [1] as a backend. We disable XLA\textsuperscript{3} and sample the collocation points randomly. All the results are available on GitHub\textsuperscript{4} and fully reproducible, with a global random seed of 1234. We use Glorot uniform initialization [3, Chapter 8]. “Error” refers to the $L^2$-relative error, and “Time” (in seconds) stands for the training time.

For MO-TPINNs, we set the weights in (3.10) as:

$$\omega_1 = 1 \quad \omega_j = 1000, \quad j = 1, \cdots, k.$$

For each case, we compare both V-TPINNs and MO-TPINNs. Each subsection is intended to bring a novelty concerning solving operator equations with stochastic data:

- Subsection 6.2 - 1D Poisson: Higher order moments $k = \{1, \cdots, 4\}$;
- Subsection 6.3 - 1D Schrödinger: Non-linear operator;
- Subsection 6.4 - 2D Helmholtz: Two-dimensional problem with oscillatory behavior;
- Subsection 6.5 - 1D Heat: Time-domain operator.

For the sake of simplicity, we summarize the parameters and hyper-parameters for TPINNs for each case in Table 6.1.

\textsuperscript{2}https://deepxde.readthedocs.io/
\textsuperscript{3}https://www.tensorflow.org/xla
\textsuperscript{4}https://github.com/pescap/TensorPINNs
| Case            | learning rate | width | depth | epochs | N     | N_{test} | σ  |
|----------------|---------------|-------|-------|--------|-------|----------|----|
| 1D Poisson     | 10^{-3}       | 50    | 4     | 10000  | 4000  | 1000     | tanh |
| 1D Schrödinger | 10^{-3}       | 50    | 4     | 10000  | 4000  | 1000     | tanh |
| 2D Helmholtz   | 10^{-2}       | 350   | 2     | 10000** | 5000  | 5000     | sin  |
| 1D Heat        | 10^{-3}       | 20    | 3     | 15000  | 4000  | 4000     | tanh |

Table 6.1: Overview of the parameters and hyper-parameters for each case; *10^{-4} for MO-TPINNs; **15000 for covariance kernels in Subsection 6.4.2.

### 6.2. Poisson 1D.

To begin with, we consider the Laplace equation in $D := [0, 1]$. For $k \in \mathbb{N}$, we seek $u \in L^k(\Omega, \mathbb{P}, X)$ such that

$$-\Delta u(\omega) = f_D(w) \quad \text{and} \quad u(\omega)|_\Gamma = 0 \quad \mathbb{P}\text{-a.e. } \omega \in \Omega$$

with

$$f_D(\omega) = xe^{\mu(\omega)}, \quad \int_D := x, \quad \omega \in \Omega, \quad \mu > 0.$$

This problem can be cast as (2.3) with $A : X = H^1(D) \to Y = L^2(D)$ [21, Remark 3.2]. Acknowledge that for any $\omega \in \Omega$:

$$u(\omega) = \pi e^{\mu(\omega)}, \quad \pi(x) := -\frac{1}{6}x(x^2 - 1).$$

As a consequence, there holds that:

$$(6.2) \quad A_D^{(k)} \mathcal{M}^k[u] = \mathcal{M}^k[f_D] = c_\sigma \int_D^{(k)} \quad \text{with} \quad c_\sigma := \mathcal{M}^k[e^{\mu(\omega)}] = e^{\frac{1}{2}k^2\sigma^2},$$

yielding

$$\mathcal{M}^k[u] = c_\sigma \pi^{(k)}.$$

Notice that $k = 1$ simplifies to $A_D \pi = \int_D$. We enforce the Dirichlet BCs throughout the transformation:

$$(6.3) \quad \hat{\Sigma}^k = \left( \prod_{i=1}^{k} x_i(x_i^2 - 1) \right) \Sigma^k,$$

and solve (6.2) for $k = 1, \cdots, 4$ and $\sigma = 1$ via TPINNs. In Figure 6.1 we represent $\text{diag}(\Sigma^k_0)$. In the same fashion, we represent the pointwise residual error in Figure 6.2.

In Table 6.2, we summarize the results for TPINNs. We remark that the training and test losses are increasing with $k$. Surprisingly, the error is low and remains stable with $k$. TPINNs provide a precise approximation with $N = 4000$ training points and almost identical neural networks (see $|\Theta|$). However, as expected, the curse of dimensionality stems from higher-order derivatives, inducing a strong increase in training times, e.g., 5246.1s., i.e. 1 hour and 27 minutes for $k = 4$. According to these results, TPINNs prove to be an efficient and robust technique for approximating the statistical moments. TPINNs deliver a surprisingly precise approximation to the tensor equation.

In the same fashion, we represent the results for MO-TPINNs in Table 6.3. Here, the method shows controlled computational cost, at the expense of adding more terms to the function loss, and learning extra variables. We observe that training times remain stable with $k$. However, acknowledge that losses and errors grow with $k$. For $k = 4$, MO-TPINNs yield a relative error of 23.4%. Notice in (6.1) that MO-TPINNs fail at representing accurately the diagonal terms.
6.3. Stationary 1D Schrödinger. In this case, we add a cubic non-linear term to Subsection 6.2. For any \( \lambda \neq 0 \) and \( \kappa \in \mathbb{R} \), we consider the one-dimensional (non-linear) time-harmonic Schrödinger equation [25]:

\[
-\partial_x^2 u(\omega) - \lambda u^3(\omega) - \kappa^2 u(\omega) = f_D(\omega) \quad \text{for} \quad x \in D = (0,1) \quad \text{with} \quad u(\omega)|_T = 0 \quad \mu\text{-a.e.} \in \Omega.
\]
We set $\lambda = 1$ and $\kappa = 0$, and reuse the manufactured solution $u(\omega)$ as in (6.1). Thus, we have the source term $f_D(\omega) = \mathcal{I}_D e^{\mu(\omega)}$ with

$$\mathcal{I}_D(x) = x - \lambda \bar{\pi}^3(x) \quad \text{in} \quad D.$$  

Notice that for $k = 1$, (2.4) yields $A_D \bar{\pi} = \mathcal{I}_D$. For $k = 2$, we set $S: u \mapsto u^3$. There holds that for $x, y \in D$:

$$(A_D \otimes A_D)\Sigma(x, y) = (-x^2 \sigma - \lambda S^3) \otimes (-\partial^2_{yy} - \lambda S^3)\Sigma(x, y)$$

$$= \partial^2_{xx} \Sigma(x, y) + \partial^2_{xy} \Sigma^3(x, y) + (\partial^2_{yy} \Sigma)^3(x, y) + \Sigma^6(x, y).$$

We set:

$$(6.5) \quad \Sigma_D(x, y) = c_\sigma v(x) w(y)$$

with $v = w = \bar{\pi}$, and $c_\sigma$ in (6.2). We aim at obtaining the manufactured right-hand side corresponding to (6.5). First, acknowledge that:

$$\partial^2_{xx} v^3(x) = \partial_x (3 \partial_x v(x) v(x))$$

$$= 3 \partial^2_{xx} v(x) v(x) + 3(\partial_x v(x))^2$$

$$= 3 \left[-x v(x) + \left(-\frac{x^2}{2} + \frac{1}{6}\right)^2\right].$$

Second,

$$\partial^2_{xx} \partial^2_{yy} \Sigma(x, y) = c_\sigma xy, \quad (\partial^2_{yy} \Sigma(x, y))^3 = -c_\sigma^3 v(x)^3 y^3 \quad \text{and} \quad \Sigma^6(x, y) = c_\sigma^6 v(x)^3 w(y)^3.$$ 

As a consequence:

$$(A_D \otimes A_D)\Sigma(x, y) = c_\sigma xy + 3c_\sigma \left[-x v(x) + \left(-\frac{x^2}{2} + \frac{1}{6}\right)^2\right] w(y)^3 - c_\sigma^3 v(x)^3 y^3 + c_\sigma^6 v(x)^3 w(y)^3$$

$$=: C_D(x, y) \equiv \mathcal{M}^2[f_D].$$

We use the transformation in (6.3) and apply TPINNs to (6.5) with the parameters in Table 6.1. As regards MO-PINNs we set:

$$(6.6) \quad \begin{cases} 
-\partial^2_{xx} V_0 - \lambda V_0^3 = C_D \\
-\partial^2_{yy} V_1 - \lambda V_1^3 = V_0.
\end{cases}$$

We represent $\text{diag}(\Sigma_\theta)$ and the pointwise error in Figure 6.3 for both TPINN architectures. On the left-hand figure, we portray the training collocation points. Both models achieved to manage and learn the non-linearity. To our knowledge, this is the first time that non-linear tensor operator equation is solved numerically. TPINNs give an accurate solution, with pointwise error being lesser than $2 \times 10^{-5}$ (resp. $4 \times 10^{-4}$) for V-TPINN (resp. MO-TPINN). To go further, the results are summarized in Table 6.4. We notice that all models have low training errors and generalize well ($\mathcal{L}_\theta \approx \mathcal{L}_\theta^{\text{test}}$). V-TPINN gives a more precise solution than MO-TPINN despite showing similar test loss. We remark that both TPINNs provide a highly accurate approximation in less than 150 seconds, which is remarkable.

| k | $\mathcal{L}_\theta$   | $\mathcal{L}_\theta^{\text{test}}$ | Error       | Time (s) | $|\Theta|$ |
|---|------------------------|-------------------------------------|-------------|----------|-----------|
| 1 | $6.21 \times 10^{-7}$   | $6.26 \times 10^{-7}$              | $2.03 \times 10^{-4}$ | 36.6     | 7801      |
| 2 | $1.36 \times 10^{-2}$   | $1.35 \times 10^{-2}$              | $1.10 \times 10^{-2}$ | 48.9     | 7902      |
| 3 | $1.07 \times 10^{-1}$   | $1.32 \times 10^{-1}$              | $4.86 \times 10^{-2}$ | 67.9     | 8003      |
| 4 | $2.00 \times 10^{3}$    | $6.65 \times 10^{3}$               | $2.34 \times 10^{-1}$ | 88.5     | 8104      |

Table 6.3: Poisson 1D. Overview of the results for MO-TPINNs.

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Fig. 6.3: Schrödinger 1D. V-TPINN (up) and MO-TPINN (bottom) for $\Sigma_0^2$. We represent the solution along with the training collocation points (left). The exact solution is represented (center) and the pointwise difference between the TPINN and exact solution (right).

| k  | Architecture | $L_2$  | $L_2^{\text{test}}$ | Error   | Time (s) | $|\Theta|$ |
|----|--------------|--------|---------------------|---------|----------|---------|
| 1  | -            | $9.41 \times 10^{-7}$ | $9.42 \times 10^{-7}$ | $2.42 \times 10^{-4}$ | 35.9     | 7801    |
| 2  | V-TPINN      | $4.49 \times 10^{-5}$ | $4.97 \times 10^{-5}$ | $9.71 \times 10^{-4}$ | 146.8    | 7851    |
| 2  | MO-TPINN     | $4.73 \times 10^{-5}$ | $5.54 \times 10^{-5}$ | $1.23 \times 10^{-2}$ | 65.4     | 7902    |

Table 6.4: Schrödinger 1D. Overview of the results.

6.4. Helmholtz equation in two dimensions. We aim at verifying that TPINNs can be applied to more complex problems, particularly, for $d > 1$. We consider the solution of the Helmholtz equation over $D := [0,1]^d$, $d = 2$ with $n \in \mathbb{N}$ and $\kappa := 2\pi n$ such that

$$-\Delta u(\omega) - \kappa^2 u(\omega) = f_D(\omega) \quad \text{with} \quad u(\omega)|_{\Gamma} = 0 \quad \text{P-a.e.} \ \omega \in \Omega.$$ 

For $k = 1$, we set

$$E[f_D] = \mathcal{F}_D(x, y) := \kappa^2 \sin(n\pi x)\sin(n\pi y),$$

and use the transformation $(x, y) \rightarrow x(x - 1)y(y - 1)$ to enforce the BCs.

Let us focus now on $k = 2$ and $\Sigma = M^2[u]$. One has that:

$$(A_D \otimes A_D)\Sigma = (-\Delta_{x_1} - \kappa^2) \otimes (-\Delta_{x_2} - \kappa^2)\Sigma$$

$$= \Delta_{x_1}\Delta_{x_2}\Sigma + \kappa^2 \Delta_{x_1}\Sigma + \kappa^2 \Delta_{x_2}\Sigma + \kappa^4 \Sigma.$$ 

Boundary conditions are enforced via the transformation:

$$\Sigma := x(x - 1)y(y - 1)z(z - 1)t(t - 1)\Sigma.$$  (6.7)
Lastly, MO-TPINNs in (3.6) rewrite as:

\[
\begin{align*}
-\Delta x_1 V_0 - \kappa^2 V_0 &= C_D, \\
-\Delta x_2 V_1 - \kappa^2 V_1 &= V_0.
\end{align*}
\] (6.8)

We apply TPINNs with the parameters in Table 6.1 for separable right-hand side, and exponential covariance kernel.

6.4.1. Separable right-hand side. We set \( x_1 = (x, y) \), \( x_2 = (z, t) \) and define the following separable right-hand side:

\[
C_D(x, y, z, t) := \kappa^4 \sin(n\pi x) \sin(n\pi y) \sin(n\pi z) \sin(n\pi t) = f_D \otimes f_D
\] (6.9)

with \( f_D \) in (6.4). We represent \( \text{diag}(\Sigma^k) \) for V-TPINNs and MO-TPINNs in Figure 6.4 and Figure 6.5, respectively. As in previous subsections, TPINNs yield an accurate approximation to \( \text{diag}(\Sigma^k) \), with pointwise error lesser than 0.04 (resp. 0.06) for V-TPINNs (resp. MO-TPINNs). It is worth to mention that \( \|\Sigma\|_{L^\infty(D(k))} = 1 \).

![Fig. 6.4: Helmholtz 2D: Solution and pointwise error of V-TPINN for \( \text{diag}(\Sigma^k) \) and a separable right-hand side.](image1)

![Fig. 6.5: Helmholtz 2D: Solution and pointwise error of MO-TPINN for \( \text{diag}(\Sigma^k) \) and a separable right-hand side.](image2)

In Table 6.5, we give further details on performance. We remark that: (i) the models train and generalize well; (ii) losses and error for both TPINNs are similar, and around 100 times less precise than for \( k = 1 \). Furthermore, MO-TPINNs yield similar training time to case \( k = 1 \), for an error of 7.09%, outperforming V-TPINNs in this case: the error for MO-TPINNs is 22% higher than for V-TPINNs, for a 5-fold faster training.
6.4.2. Exponential covariance kernel. Separable right-hand sides allow to use a manufactured solution. Once convergence is verified, application of TPINNs to general right-hand side is straightforward. We introduce the squared exponential (Gaussian) and 1-exponential covariance functions $f_D \sim \mathcal{GP}(f_D, C_D)$ [20, Fig. 2] with $f_D$ in (6.4) and (6.10) 

$$C_D(x_1, x_2) = \sigma^2 \exp \left(-\frac{|x - z|^2}{2\lambda}\right)$$

and

$$C(x_1, x_2) = \sigma^2 \exp \left(-\frac{|x - z|^2}{2\lambda}\right)$$

for $x_1 = (x, y)$, $x_2 = (z, t)$, $\sigma \in \mathbb{R}$ and $\lambda > 0$. We apply TPINNs again for $\sigma = \kappa^2$ and $\lambda = 5$. To begin with, in Figure 6.6 we represent $\text{diag}(C_D)$ for the three right-hand sides considered.

![Figure 6.6: Helmholtz 2D: Plot of $\text{diag}(C_D)$ defined in (6.9) and (6.10).](image)

Next, we plot the diagonal of V-TPINN and MO-TPINN for the Gaussian kernel in Figure 6.7. Remark that the solutions differ. Likewise, the diagonal for exponential kernel is represented in Figure 6.8. This time, the solutions have a more similar pattern. To give a further insight on these simulations, we summarize the results in Table 6.6. First, we remark that V-TPINNs failed to train in the Gaussian case ($L_\theta = 1.34 \times 10^3$ while $L_{\text{test}} = 1.08 \times 10^6$). This behavior was quite unexpected, as Gaussian kernels are smoother than 1-exponential kernels. Training losses are $\sim 10^2$ for exponential kernel, as compared to $\sim 10^4$ for separable right-hand sides in Table 6.5: training loss is sensitive to the right-hand side.

| k | Architecture | $L_\theta$ | $L_{\text{test}}$ | Error | Time (s) | $|\Theta|$ |
|---|--------------|------------|------------------|------|---------|-------|
| 1 | -            | $5.93 \times 10^{-4}$ | $5.41 \times 10^{-4}$ | $4.52 \times 10^{-4}$ | 159.3 | 124251 |
| 2 | V-TPINN     | $1.33 \times 10^1$   | $1.74 \times 10^1$   | $5.82 \times 10^{-2}$ | 814.2 | 124951 |
| 2 | MO-TPINN    | $3.59 \times 10^1$   | $4.05 \times 10^1$   | $7.09 \times 10^{-2}$ | 147.3 | 125302 |

Table 6.5: Helmholtz 2D: Overview of the results for a simple right-hand side.

| k | Architecture | Gaussian | Exponential |
|---|--------------|----------|-------------|
| 2 | V-TPINN     | $1.34 \times 10^{-3}$ | $2.13 \times 10^{-3}$ |
| 2 | MO-TPINN    | $5.66 \times 10^{-3}$ | $1.32 \times 10^{-3}$ |

Table 6.6: Helmholtz 2D: Overview of the results for exponential covariance kernels.
6.5. Heat equation. To finish, we apply the scheme to a time dependent operator. We consider the heat equation in \([0, L] \times [0, T]\):

\[
\partial_t u(\omega) - a \Delta u(\omega) = f_D(\omega) \quad \text{with} \quad u(\omega)|_{\Gamma} = 0 \quad \text{and} \quad u(\omega, t = 0) = \sin(n \pi x) \quad \mathbb{P}\text{-a.e.} \ \omega \in \Omega.
\]

wherein we set \(L = T = n = 1\) and \(a = 0.4\). We consider the exact solution for \(k = 1\) with \(\mathbb{E}[f] = 0\):

\[
\mathbb{E}[u] = \overline{u}(x, t) = \sin(n \pi x / L)e^{-n \pi^2 a t}
\]

and apply the following transformation:

\[
\hat{u}(x, t) = \sin(n \pi x)e^{-n \pi^2 a t} + tu(x, t).
\]

6.5.1. Separable right-hand side. For \(k = 2\), we use the following manufactured solution:

\[
\Sigma(x, t, y, z) = \overline{u}(x, t)\overline{u}(y, z).
\]
\[ \Sigma(x, t, y, t) = e^{-\pi^2 a_x^2} e^{-\pi^2 a_z^2} \sin(\pi x) \sin(\pi z) \]

for \( a = 0.4 \) and notice that:

\[
\begin{align*}
(A_D \otimes A_D) \Sigma &= (\partial_t - a \Delta_x)(\partial_x - a \Delta_y) \Sigma \\
&= \partial_t \partial_x \Sigma - a \partial_x \Delta_y \Sigma - a \partial_x \partial_x \Sigma + a^2 \Delta_x \Delta_y \Sigma \\
&= \partial_t^2 \Sigma - a \partial^2_{xy} \Sigma - a \partial^2_{xx} \Sigma + a^2 \partial^4_{xxyy} \Sigma.
\end{align*}
\]

We set the transformation:

\[
(6.13) \quad \tilde{\Sigma}(x, t, y, z) = e^{-\pi^2 t} e^{-\pi^2 z} \left( \sin(\pi x) \sin(\pi z) + t \Sigma(x, t, y, z) \right).
\]

For the MO-TPINNs, one has that:

\[
(6.14) \quad \begin{cases} 
- \partial_t V_0 - \partial^2_{xx} V_0 = C_D, \\
- \partial_z V_1 - \partial^2_{yy} V_1 = V_0.
\end{cases}
\]

with \( C_D = 0 \) in this case (see definition in Subsection 6.4.2 for the exponential case.) We solve the problem with parameters in Table 6.1, and sum up results in Table 6.7. We remark that the neural nets train well and supply accurate solutions in a few minutes. It is worthy to notice that V-TPINN (resp. MO-TPINN) yields a solution with relative error of \( 8.87 \times 10^{-4} \) (resp. \( 6.60 \times 10^{-4} \)) despite being trained over nets with less than 1000 trainable parameters. This demonstrates the learning capacity of PINNs and TPINNs.

| k | Architecture | \( \mathcal{L}_a \) | \( \mathcal{L}^{\text{stat}}_a \) | Error | Time (s) | \(|\Theta|\) |
|---|---|---|---|---|---|---|
| 1 | - | 2.15 \times 10^{-8} | 2.05 \times 10^{-8} | 1.84 \times 10^{-5} | 49.8 | 921 |
| 2 | V-TPINN | 1.16 \times 10^{-5} | 1.27 \times 10^{-5} | 8.87 \times 10^{-4} | 226.9 | 961 |
| 2 | MO-TPINN | 1.02 \times 10^{-6} | 1.03 \times 10^{-6} | 6.40 \times 10^{-3} | 74.6 | 982 |

Table 6.7: Heat 1D: Overview of the results for a simple right-hand side.

**6.5.2. Exponential covariance kernel.** Next, we set the Gaussian and 1-exponential covariance kernels for \( x_1 = (x, t) \) and \( x_2 = (y, z) \) as:

\[
C_D(x_1, x_2) = \sigma^2 \exp \left( -\frac{|x-y|^2}{2\lambda} - 2(t-z) \right) \quad \text{and} \quad C_D(x_1, x_2) = \sigma^2 \exp \left( -\frac{|x-y|^2}{2\lambda} - 2(t-z) \right)
\]

respectively, with \( \sigma = 10 \) and \( \lambda = 5 \). Acknowledge that TPINNs do not generalize as well as in previous sections, despite delivering low test losses of \( 7.71 \times 10^{-2} \) (resp. \( 4.80 \times 10^{-4} \)) for V-TPINN (resp. MO-TPINN). It is important to notice that in this case, MO-TPINNs leads to an approximation with a lower test error and training time (by a factor of 3). To finish, we represent \( \text{diag}(\Sigma_\theta) \) for both covariance kernels in Figure 6.9 and Figure 6.10. Notice that the difference between solutions is low but noticeable in Figure 6.9, while being imperceptible in Figure 6.10. It is again interesting to notice that Gaussian kernel is harder to train that its 1-exponential counterpart.

**7. Conclusion.** In this work, we introduced TPINNs to solve operator equations with stochastic right-hand-side. We considered two architectures for TPINNs, namely V-TPINNs and MO-TPINNs, both showing efficient performance for across a variety of operators. We included a bound for the generalization error for V-PINNs in Theorem 4.1, paving the way toward robust TPINNs and aiding in better understanding their behavior. Our numerical experiments
proved that TPINNs are a powerful technique, applicable to challenging problems. It is interesting to notice that none of them consistently outperformed the other, justifying their introduction. Although a promising approach to overcoming the curse of dimensionality for tensor operator equations, V-TPINNs (resp. ML-TPINNs) have shown an increasing cost with k due to automatic differentiation (resp. difficulties inherent to training), opening research pathways towards more efficient schemes.
Further work includes coupling the results in Section 4 with shift theorems [28] to supply complete convergence bounds of the behavior of PINNs. Also, TPINNs could be applied to UQ for small amplitude perturbed random domains [14, 9]. Alongside, hard BCs are no longer applicable for complex geometries, justifying the use of soft BCs TPINNs.

Finally, MO-TPINNs proved to be a surprisingly fast technique. In our opinion, improving training is a promising research area. This could involve: (i) optimizing weights during training, for example through learning rate annealing [33]; or (ii) conducting hyperparameter optimization training is a promising research area. This could involve: (i) optimizing weights during training, for example through learning rate annealing [33]; or (ii) conducting hyperparameter optimization training is a promising research area. This could involve: (i) optimizing weights during training, for example through learning rate annealing [33]; or (ii) conducting hyperparameter optimization training is a promising research area. This could involve: (i) optimizing weights during training, for example through learning rate annealing [33]; or (ii) conducting hyperparameter optimization training is a promising research area. 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This could involve: (i) optimizing weights during training, for example through learning rate annealing [33]; or (ii) conducting hyperparameter optimization training is a promising research area. This could involve: (i) optimizing weights during training, for example through learning rate annealing [33]; or (ii) conducting hyperparameter optimization trainin...
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