Power Method, Inverse Power Method and Shifted Inverse Power Method Neural Networks for Solving Eigenvalue Problems of Linear Operators

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Abstract
In this article, we propose three methods Power Method Neural Network (PMNN), Inverse Power Method Neural Network (IPMNN) and Shifted Inverse Power Method Neural Network (SIPMNN) combined with power method, inverse power method and shifted inverse power method to solve eigenvalue problems with the dominant eigenvalue, the smallest eigenvalue and the smallest zero eigenvalue, respectively. The methods share similar spirits with traditional methods, but the differences are the differential operator realized by Automatic Differentiation (AD), the eigenfunction learned by the neural network and the iterations implemented by optimizing the specially defined loss function. We examine the applicability and accuracy of our methods in several numerical examples in high dimensions. Numerical results obtained by our methods for multidimensional problems show that our methods can provide accurate eigenvalue and eigenfunction approximations.

1. Introduction

Recently, neural network has achieved remarkable success in solving Partial Differential Equations (PDEs). Especially, deep Ritz method proposed by E and Yu [1] and Physcis-Informed Neural Netowrk (PINN) proposed by Raissi et al.[2] have attracted widespread attention. With the unprecedented availability of computational power, extensive researches have been done on developing neural network for solving PDEs which can be traced back to 1990s [3–5]. These days, neural network has led to some remarkable results for solving a variety of problems, including heat transfer problems [6], finance [7], uncertainty quantification [8–10], inverse problems [11, 12] and so on.

However, seldom researches focus on using neural network to solve the eigenvalue problems. Deep Ritz method [1] first proposed using the Rayleigh quotient to solve the smallest eigenvalue problems. The authors transformed the original eigenvalue problem to the function which is known as the Rayleigh quotient using the variational principle for the smallest eigenvalue. The main idea of the Rayleigh quotient is the fact that it gives the range of eigenvalues of the operator. Then, the authors minimized the function and got the smallest eigenvalue and the associated eigenfunction which is expressed by the neural network. Following the main idea of the Rayleigh quotient, some researchers proposed directly using the Rayleigh quotient to construct the function without variation and using PINN to solve this kind of function [13, 14].

Some other researchers [15, 16] proposed adding one or two regularization terms into the loss function. Therefore, when minimizing the loss function, the neural network will try to learn the smallest eigenvalue. Moreover, Han et al. [17] formulated the eigenvalue problem by Forward-Backward Stochastic Differential Equations (FBSDE) using the diffusion Monte Carlo method, where the loss function minimized the eigenvalue, eigenfunction and the scaled gradient of the eigenfunction.

Unfortunately, these methods are difficult to be used in practical applications. Especially, the methods of adding regularization terms into the loss function often can not find the convergence point in the learning curve of a neural network. Because the regularization term $e^{-\lambda + c}$ relies heavily on the constant $c$. In addition, all methods discussed above are trying to minimize the eigenvalue $\lambda$, which will be expected to result in a bad result. Because the optimization of the neural network prefers to minimize the loss to zero loss which is contrasted to the eigenvalue which may not be zero. Furthermore, because there are many items in loss function, it is also problematic for the neural network to
PMNN, IPMNN and SIPMNN

balance the weight of them. Moreover, the researches only focus on solving for the smallest eigenvalue and does not possess the ability of solving for the dominant eigenvalue.

Therefore, we try to find some new methods to overcome the shortcomings of directly minimizing eigenvalue. To the best of the authors’ knowledge, neural network, in conjunction with power method, inverse power method and shifted inverse power method, are still barely explored. In this work, we propose three new methods PMNN, IPMNN and SIPMNN to solve high-dimensional eigenvalue problems with the dominant eigenvalue, the smallest eigenvalue and the smallest zero eigenvalue, respectively. In similar spirits of traditional methods, our methods focus on linear differential operators and iteratively approximate the real eigenvalue and eigenfunction. However, compared with traditional methods, our methods have some differences with them. Specifically, instead of discretizing the differential operator to a matrix, we use AD [18] to represent it. Then conventional methods discretize the eigenfunction to one eigenvector, but our methods use the neural network to learn the eigenfunction. Although our methods also use eigenvector to represent the eigenfunction, it just is used in the training stage. Another difference is the iterations which is implemented by optimizing specially defined loss function.

This article is organized as follows, in Section 2, we introduce the basic assumptions of the problems we focus on and retrospect the main idea of power method and inverse power method. In Section 3, we propose three new methods PMNN, IPMNN and SIPMNN. In Section 4, numerical examples and results are presented. Finally, the conclusions and future work are provided in Section 5.

2. Preliminaries

2.1. Eigenvalue Problems

Let $H$ be a Hilbert space where the inner product for $u, v \in H$ is $\langle u, v \rangle$. Let $A \in O(H)$ be an operator. Let $A^*$ be the adjoined operator [19] defined by $\langle A^* u, v \rangle = \langle u, Av \rangle \ \forall u, v \in H$. Then $A$ is said to be self-adjoint if $A = A^*$.

Lemma 2.1. Let $H$ be a Hilbert space. Let $A \in O(H)$ be a self-adjoint operator. Then all eigenvalues of $A$ are real.

In this work, we focus on self-adjoint operators $L$ with the dominant eigenvalue or the smallest eigenvalue. Suppose that we have PDE as follows,

\[
\begin{cases}
Lu = \lambda u, & \text{in } \Omega, \\
Bu = g, & \text{on } \partial \Omega,
\end{cases}
\]

where the domain $\Omega \subset \mathbb{R}^d$, $L$ and $B$ are two differential operators acting on the functions defined in the interior of $\Omega$ and on the boundary $\partial \Omega$, respectively, and $(u, \lambda)$ is an eigenpair of the operator $L$ which is defined as: $(u, \lambda) \ s.t. \ \lambda \in \mathbb{R}$, where $u$ is the eigenfunction of $L$ and $\lambda$ is the corresponding eigenvalue.

To estimate the dominant or smallest eigenvalue of the operator $L$, the basic assumptions are given as follows,

- $L$ is a self-adjoint operator which means that all eigenvalues of $L$ are real;
- $L$ is a linear operator;
- $L$ has the dominant or smallest eigenvalue, and $(u, \lambda_{\text{max}})$ or $(u, \lambda_{\text{min}})$ is the corresponding eigenpair;
- If $L$ has a lots eigenvalues and $\lambda_1$ is the dominant eigenvalue, the eigenvalues can be listed as follows, $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_n| \geq \cdots$;
- If $L$ has a lots eigenvalues and $\lambda_1$ is the smallest eigenvalue, the eigenvalues can be listed as follows, $0 < |\lambda_1| < |\lambda_2| \leq |\lambda_3| \leq \cdots \leq |\lambda_n| \leq \cdots$.

Over the past century, many conventional methods have been used to numerically solve the Equation (1), for example, finite difference method [20, 21], finite element method [22, 23], finite volume method [24, 25] and spectral method [26, 27]. The key idea of these methods is to construct a matrix, then use power method or inverse power method to solve the dominant eigenvalue or smallest eigenvalue. Therefore, We will introduce the power method and inverse power method [28] in a form of a matrix in later subsections.
2.2. Power Method

The power method is one of the most basic and often-used algorithms in numerical linear algebra. It is used to find the largest eigenvalue (in absolute value) and the corresponding eigenvector of a matrix. Such an eigenvalue is called a dominant eigenvalue.

Suppose $A \in \mathbb{R}^{n \times n}$ is a diagonalizable $n \times n$ matrix having $n$ eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, with $\lambda_1$ being the dominant eigenvalue and the eigenvalues can be listed as $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_n| \geq 0$. The power method can be used to find $\lambda_1$ and its associated eigenvector. Let $X \in \mathbb{R}^{n \times n}$ be the matrix of its eigenvectors $x_i$ corresponding to $\lambda_i$, for $i = 1, 2, \ldots, n$. And $x_1, x_2, \ldots, x_n$ are linearly independent.

Since $x_1, x_2, \ldots, x_n$ are linearly independent set, there exists constants $c_1, c_2, \ldots, c_n$ such that an arbitrary vector $x \in \mathbb{R}^{n \times 1}$ can be uniquely expressed as

$$x = c_1 x_1 + c_2 x_2 + \cdots + c_n x_n.$$  \hspace{1cm} (2)

Suppose $c_1 \neq 0$ is the constraint to the vector $x$. Now, let's multiply both sides by $A$:

$$Ax = c_1 Ax_1 + c_2 Ax_2 + \cdots + c_n Ax_n.$$  \hspace{1cm} (3)

Since $Ax_i = \lambda_i x_i$, we will have

$$Ax = c_1 \lambda_1 x_1 + c_2 \lambda_2 x_2 + \cdots + c_n \lambda_n x_n.$$  \hspace{1cm} (4)

Continue to multiply $A$ with $(k - 1)$ times, then we can get

$$A^k x = c_1 \lambda_1^k x_1 + c_2 \lambda_2^k x_2 + \cdots + c_n \lambda_n^k x_n$$

$$= c_1 \lambda_1^k [x_1 + \frac{c_2}{c_1} \frac{\lambda_2}{\lambda_1} x_2 + \cdots + \frac{c_n}{c_1} \frac{\lambda_n}{\lambda_1} x_n].$$  \hspace{1cm} (5)

Since $\lambda_1$ is the dominant eigenvalue ($|\lambda_1| > |\lambda_i|$ for $2 \leq i \leq n$), the ratio $\lambda_2/\lambda_1, \lambda_3/\lambda_1, \ldots, \lambda_n/\lambda_1$ are fewer than 1 in magnitude, hence for a sufficiently large $k$, $\lambda_1^k$ is significantly larger than $\lambda_i^k$, then the ratio $\lambda_1^k/\lambda_i^k$ approaches 0 as $k \to \infty$. Thus, the term $c_1 \lambda_1^k x_1$ dominates the expression for $A^k x$ for large enough value of $k$. If we normalize $A^k x$, then we can get $u = (A^k x)/\|A^k x\| \approx (c_1 \lambda_1^k x_1)/\|c_1 \lambda_1^k x_1\|$, which is a scalar multiple of $x_1$. Thus, $u$ is a unit eigenvector corresponding to the dominant eigenvalue $\lambda_1$.

Finally, we get $Au \approx \lambda_1 u$. Therefore, $\|Au\|$ approximates $|\lambda_1|$. The sign of $\lambda_1$ is determined by checking whether $Au$ is in the same direction as $u$ or in the opposite direction. The implementation details of power method can also be seen in Algorithm 1.

2.3. Inverse Power Method

The inverse power method is also one of the most basic and often-used algorithms in numerical linear algebra. It follows the main idea of power method to find a smallest eigenvalue (in absolute value too) and the corresponding eigenvector of a matrix.

Suppose $A \in \mathbb{R}^{n \times n}$ is a diagonalizable $n \times n$ matrix having $n$ eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, with $\lambda_1$ being the smallest eigenvalue and the eigenvalues can be listed as $0 < |\lambda_1| < |\lambda_2| \leq |\lambda_3| \leq \cdots \leq |\lambda_n|$. Therefore, $A$ is a nonsingular matrix and the inverse of it $A^{-1}$ exists. The inverse power method can be used to find $\lambda_1$ and an associated eigenvector. Let $X \in \mathbb{R}^{n \times n}$ be the matrix of its eigenvectors $x_i$ corresponding to $\lambda_i$, for $i = 1, 2, \ldots, n$. And $x_1, x_2, \ldots, x_n$ are linearly independent.

The same as power method, an arbitrary vector $x \in \mathbb{R}^{n \times 1}$ can be uniquely expressed as Equation (2). And $c_1 \neq 0$ is also the constraint to the vector $x$. Since $0 < |\lambda_1| < |\lambda_2| \leq |\lambda_3| \leq \cdots \leq |\lambda_n|$, then we can get $|1/\lambda_1| > |1/\lambda_2| \geq |1/\lambda_3| \geq \cdots \geq 1/\lambda_n > 0$ and $1/\lambda_1, 1/\lambda_2, \ldots, 1/\lambda_n$ are the eigenvalues of the matrix $A^{-1}$. To solve $Ax = \lambda x$, we can transform it to $A^{-1} x = 1/\lambda x$. Hence, the problems has been transformed to solve the dominant eigenvalue of the matrix $A^{-1}$. The implementation details of inverse power method can also be seen in Algorithm 2.

3. Methodologies

In this work, we aim to solve the eigenvalue problems without constructing any matrix. By doing this, we propose two architecture to solve the dominant eigenvalue problems and the smallest eigenvalue problems, that is PMNN and IPMNN which follow the main ideas of power method and inverse power method.
Algorithm 1: Power Method for Finding the Dominant Eigenvalue of a Square Matrix

Given \( A \in \mathbb{R}^{n \times n} \) a \( n \times n \) matrix.

**Step 1:** Choose an arbitrary unit vector \( u_0 \in \mathbb{R}^{n \times 1} \).

**Step 2:** Give the maximum number of iterations \( k_{\text{max}} \) and the stopping criterion \( \epsilon \).

**Step 3:** Create two temporary vectors \( u_{k-1} \in \mathbb{R}^{n \times 1} \) and \( u_k \in \mathbb{R}^{n \times 1} \).

**Step 4:** Let \( u_{k-1} = u_0 \), then iterate the process as follows,

\[
\text{for } i = 1, 2, \ldots, k_{\text{max}} \text{ do}
\begin{align*}
    u_k &= A u_{k-1} , \\
    u_k &= u_k / \| u_k \| , \\
    \text{if } \| u_k - u_{k-1} \| < \epsilon \text{ then} & \\
    & \text{The stopping criterion is met, the iteration can be stopped.} \\
    \text{else} & \\
    & u_{k-1} = u_k .
\end{align*}
\]

end

Then, we can obtain the dominant eigenvalue \( \lambda \) through Rayleigh quotient.

\[
\lambda = u_k^T A u_k .
\]

Algorithm 2: Inverse Power Method for Finding the Smallest Eigenvalue of a Square Matrix

Given \( A \in \mathbb{R}^{n \times n} \) a \( n \times n \) matrix.

**Step 1:** Choose an arbitrary unit vector \( u_0 \in \mathbb{R}^{n \times 1} \).

**Step 2:** Give the maximum number of iterations \( k_{\text{max}} \) and the stopping criterion \( \epsilon \).

**Step 3:** Create two temporary vectors \( u_{k-1} \in \mathbb{R}^{n \times 1} \) and \( u_k \in \mathbb{R}^{n \times 1} \).

**Step 4:** Let \( u_{k-1} = u_0 \), then iterate the process as follows,

\[
\text{for } i = 1, 2, \ldots, k_{\text{max}} \text{ do}
\begin{align*}
    u_k &= A^{-1} u_{k-1} , \\
    u_k &= u_k / \| u_k \| , \\
    \text{if } \| u_k - u_{k-1} \| < \epsilon \text{ then} & \\
    & \text{The stopping criterion is met, the iteration can be stopped.} \\
    \text{else} & \\
    & u_{k-1} = u_k .
\end{align*}
\]

end

Then, we can obtain the smallest eigenvalue \( \lambda \) through Rayleigh quotient.

\[
\lambda = u_k^T A u_k .
\]

3.1. Enforcement of Boundary Conditions

As we know, in lack of proper restrictions to boundary conditions, PDEs system may have infinitely many solutions [29]. Therefore, it is important for not only numerical methods but also neural networks to enforce exactly the boundary conditions. Unlike PINN using an additional residual loss to implement the boundary conditions, we omit the boundary conditions by enforcing the exact boundary conditions. Because one pioneering work [30] have systematically represented how to enforce the exact boundary conditions, for simplicity, we will introduce the enforcement of the Dirichlet boundary condition and the periodic boundary condition.
3.1.1. Enforcement of Dirichlet Boundary Condition

For the Dirichlet boundary condition, we can directly get the values of solutions on the boundary. The boundary condition of Equation (1) can be rewrote as follows,

$$ u(x) = g(x), \quad \forall x \in \partial \Omega. \quad (6) $$

Therefore, we can straightforward design a distance function $\phi(x)$ and $G(x)$, a smooth extension of $g(x)$ in $\Omega$.

$$ \phi(x) \begin{cases} = 0, & \forall x \in \partial \Omega, \\ \neq 0, & \forall x \in \Omega. \end{cases} \quad (7) $$

Then, suppose $N_\theta(x)$ be the output of neural networks and $u_\theta(x)$ be the learned function which has been enforced the Dirichlet boundary condition.

$$ u_\theta(x) = \phi(x)N_\theta(x) + G(x), \quad \forall x \in \Omega. \quad (8) $$

3.1.2. Enforcement of Periodic Boundary Condition

For the periodic boundary conditions, we only focus on the function without derivative like Equation (9), where $P_i$ is the period along the $i$-th direction. As for how to enforce more complex periodic boundary conditions, one can refer to [31].

$$ u(x_1, \cdots, x_i + P_i, \cdots, x_d) = u(x_1, \cdots, x_i, \cdots, x_d), \quad \forall x \in \partial \Omega. \quad (9) $$

Unlike the enforcement of the Dirichlet boundary condition to modify the output of neural networks, the enforcement of periodic boundary condition tries to modify the input before the first hidden layer of neural networks. Suppose $u$ satisfies the periodic boundary in $x_i$ direction, then the component $x_i$ in $x$ is transformed as follows,

$$ x_i \to \{ \sin(2\pi j \frac{x_i}{P_i}), \cos(2\pi j \frac{x_i}{P_i}) \}^{k}_{j=1}, \quad (10) $$

where $k$ is one hyper-parameter which can be determined by oneself. The network structure can be seen in Figure 1. As we can see in Figure 1, the component $x_i$ in $x$ is transformed by Equation (10). Then, the every components of transformed $x_i$ are fed into the neural network with other components of $x$. Obviously, the number of neurons of the neural network increases from $d$ to $(d + 2k - 1)$.

3.2. Neural Networks for Solving Eigenvalue Problems

As discussed above, we have enforced the boundary conditions. Therefore, we can omit the implication of operator $\mathbb{B}$ on boundary $\partial \Omega$ and focus on the effect of linear differential operator $\mathcal{L}$ in Equation (11).

$$ \mathcal{L}u = \lambda u, \quad \text{in} \quad \Omega. \quad (11) $$

Hence, aiming to solve Equation (11), we propose three methods to solve for dominant eigenvalue and smallest eigenvalue. In these three methods showed below, the function $u$ is expressed by neural network (which is enforced boundary conditions and is taken as a whole with the enforced boundary conditions). It is worth noting that our methods learn not only the corresponding eigenvector which is confined to a few points but also the eigenfunction. The eigenfunction $u_\theta$ expressed by neural network can predict value with any points in $\Omega$. Here $\theta$ means the parameters of neural network.

3.2.1. Power Method Neural Network

Based on the basic assumptions above and follow the main idea of power method, we propose PMNN to solve for the dominant eigenvalue and the associated eigenfunction.

Focus on the key code of Algorithm 1 which has been showed in Equation (12). In PMNN, we use the neural network to represent $u_{k-1}$ and calculate $u_k$ using Equation (13). Different from the original power method, $\mathcal{L}$ is not a matrix. It is still a differential operator realized by AD. Therefore, the term $\mathcal{L}u_{k-1}$ is a whole which is computed by AD.

$$ u_k = Au_{k-1}. \quad (12) $$
However, \( u_k \) is a vector which can be directly computed by Equation (12), it will be different with \( u_k \) in Equation (13). Although \( u_k \) in Equation (13) is still an vector, it is not possible directly assign a vector to the neural network. Therefore, to solve this problem, we construct a loss function defined in Equation (14), where \( N \) denotes that there are \( N \) components in the vector and \( i \) means the \( i \)-th component. The main idea behind this equation is that we do not need the neural network to precisely compute \( u_k \) in Equation (13) in the next step. It just needs to approximate it step by step.

\[
\text{loss}_{pmnn} = \frac{1}{N} \sum_{i=1}^{N} [u_{k-1}(i) - u_k(i)]^2.
\]  

(14)

After neural network get convergence, we can get the dominant eigenvalue and associated eigenfunction expressed by the neural network. As for the details of this method, one can refer to Algorithm 3.

### 3.2.2. Inverse Power Method Neural Network

Based on the basic assumptions above and follow the main idea of inverse power method, we propose IPMNN to solve for the smallest eigenvalue and the associated eigenfunction.

Focus on the key code of Algorithm 2 which has been showed in Equation (15). Different with PMNN, in IPMNN, we use the neural network to represent \( u_k \) in Equation (16). Because it is difficult to get the inverse operator \( \mathcal{L}^{-1} \) of the differential operator \( \mathcal{L} \). Therefore, given \( u_{k-1} \) in the last iterative step, we can directly compute \( u_k \) using neural network. Here, \( \mathcal{L} \) is also not a matrix. It is still a differential operator realized by AD. Hence, the term \( \mathcal{L}u_k \) is a whole which is computed by AD.

\[
\begin{align*}
    u_k &= \mathcal{L}^{-1}u_{k-1}, \\
    u_k &= \frac{u_k}{\|u_k\|}.
\end{align*}
\]  

(15)
**Algorithm 3: PMNN for Finding the Dominant Eigenvalue**

Given $N$ the number of points for training neural network, $N_{\text{epoch}}$ the maximum number of epoch and the stopping criterion $\epsilon$.

**Step 1:** Build data set $S$ for training using random sampling algorithm.

**Step 2:** Create two temporary vectors $u_{k-1} \in \mathbb{R}^{N \times 1}$ and $u_k \in \mathbb{R}^{N \times 1}$.

**Step 3:** Construct neural network with random initialization of parameters.

**Step 4:** Let $x \in \mathbb{R}^{N \times d}$ consisted by all points in data set $S$, then iterate the process as follows, for $i = 1, 2, \cdots, N_{\text{epoch}}$ do

- Input $x$ into neural network and get the output $u$ of neural network.
- Compute $\langle \nabla u_{k-1}, u_k \rangle$ using AD.
- Let $u_{k-1} = u$.
- $u_k = u_k / \|u_k\|_2$.
- $\text{loss}_{\text{pmnn}} = \frac{1}{N} \sum_{i=1}^{N} [u_{k-1}(i) - u_k(i)]^2$.
- Update parameters of neural network using optimizer.

if $\text{loss}_{\text{pmnn}} < \epsilon$ then

- Record the best eigenvalue and eigenfunction.
- $\lambda = \frac{\langle u_{k-1}, u_k \rangle}{\langle u_{k-1}, u_{k-1} \rangle}$.
- The stopping criterion is met, the iteration can be stopped.

end

$$\frac{\mathcal{L} u_k}{\| \mathcal{L} u_k \|_2} = u_{k-1}. \quad (16)$$

However, because of the impossibleness of getting $\mathcal{L}^{-1}$, we can not directly compute $u_k$. But to follow the idea of inverse power method, $u_k$ need to equal to $\mathcal{L}^{-1} u_{k-1}$. Therefore, we construct a loss function defined in Equation (17). The main idea behind this equation is that we do not need to calculate $\mathcal{L}^{-1}$ and we use the neural network to approximate $u_k$ through $\mathcal{L} u_k$ and $u_{k-1}$. In addition, we just need the neural network to approximate it step by step.

$$\text{loss}_{\text{ipmnn}} = \frac{1}{N} \sum_{i=1}^{N} \left[ \frac{\mathcal{L} u_k(i)}{\| \mathcal{L} u_k \|_2} - u_{k-1}(i) \right]^2. \quad (17)$$

After neural network get convergence, we can get the smallest eigenvalue and the associated eigenfunction expressed by the neural network. As for the details of this method, one can refer to Algorithm 4.

### 3.2.3. Shifted Inverse Power Method Neural Network

As discussed above in the smallest eigenvalue problems, the range of eigenvalue is defined as $|\lambda| > 0$. It is common sense that inverse power method does not have the ability of solving for the smallest eigenvalue $\lambda = 0$. In addition, we also use IPMNN to solve for this special case and as expected, it does not work. Therefore, we propose SIPMNN to solve this special case.

The main idea of SIPMNN follows shifted inverse power method. Select a constant parameter $\alpha \neq 0$ and subtract $\alpha u$ from both sides of Equation (11). Then we can get Equation (18) and Equation (19), where $\mathcal{L}' = \mathcal{L} - \alpha$ and $\lambda' = \lambda - \alpha$. Therefore, the original problem can be transformed as Equation (18) and we can use IPMNN to solve for it by using Equation (19).

$$\mathcal{L} u - \alpha u = \lambda u - \alpha u, \quad \text{in } \Omega. \quad (18)$$

$$\mathcal{L}' u = \lambda' u, \quad \text{in } \Omega. \quad (19)$$
Algorithm 4: IPMNN for Finding the Smallest Eigenvalue

Given $N$ the number of points for training neural network, $N_{\text{epoch}}$ the maximum number of epoch and the stopping criterion $\epsilon$.

Step 1: Build data set $S$ for training using random sampling algorithm.

Step 2: Choose an arbitrary unit vector $u_0 \in \mathbb{R}^{N \times 1}$.

Step 3: Create two temporary vectors $u_{k-1} \in \mathbb{R}^{N \times 1}$ and $u_k \in \mathbb{R}^{N \times 1}$.

Step 4: Construct neural network with random initialization of parameters.

Step 5: Let $x \in \mathbb{R}^{N \times d}$ consisted by all points in data set $S$ and $u_{k-1} = u_0$, then iterate the process as follows, for $i = 1, 2, \ldots, N_{\text{epoch}}$ do

1. Input $x$ into neural network and get the output $u_k$ of neural network.
2. Let $u_k = u_k / \|u_k\|$.
3. Compute $\|Lu_k\|$ using AD.
4. $\text{loss}_{\text{ipmnn}} = \frac{1}{N} \sum_{i=1}^{N} \|Lu_k(i) - u_{k-1}(i)\|^2$.
5. Update parameters of neural network using optimizer.
6. $u_{k-1} = u_k / \|u_k\|$.

if $\text{loss}_{\text{ipmnn}} < \epsilon$ then

1. Record the best eigenvalue and eigenfunction.
2. $\lambda = \langle Lu_k, u_k \rangle / \langle u_k, u_k \rangle$.
3. The stopping criterion is met, the iteration can be stopped.

end

4. Numerical Experiments

In this section, we provide multi-dimensional numerical results to demonstrate the applicability and accuracy of our methods. The domain $\Omega$ with Dirichlet boundary condition is always $[0, 1]^d$. The domain $\Omega$ with period boundary condition is $[0, 2\pi]^d$. In all experiments below, we choose the Adam optimizer with initial learning rate $10^{-3}$ to minimize the loss function, and we train the neural network with a simple architecture of MLP on a server equipped with CentOS 7 system, one Intel Xeon Platinum 8358 2.60GHz CPU and one NVIDIA A100 80GB GPU. Moreover, if not otherwise specified, the activation function will be chosen as the $\tanh$ function and the random sampling algorithm will be chosen as lhs [32].

4.1. An Example of Dominant Eigenvalue Problem

To validate the performance of PMNN, we solve the following problem in $\Omega = [0, 1]^d$ with a constant coefficient $M = 100$,

$$
\begin{cases}
\Delta u + Mu = \lambda u, & \text{in } \Omega, \\
u = 0, & \text{on } \partial \Omega.
\end{cases}
$$

The dominant eigenvalue is given by $\lambda = M - d\pi^2$ and the associated eigenfunction is $u = \prod_{i=1}^{d} \sin(\pi x_i)$ where $x_i$ is the $i$-th component of $x$.

The parameters used to train PMNN for different dimensions are summarized in Table 1. For all dimensional equations, we use the different number of random sampling points $N = 10000, 20000, 50000, 10000$ for $d = 1, 2, 5, 10$. For low dimensional equations, we train PMNN with fewer epochs and smaller neural network than higher dimensional equations.

The results of PMNN are shown in Figure 2, Figure 3 and Table 2. In Figure 2, there are two lines which coincide exactly with each other means that PMNN perfectly learns the eigenfunction in one dimensional example. Figure 3 also shows the eigenfunction learned by PMNN. There are heat maps with 3 figures which show the eigenfunction of two dimensional equation. Figure on the left shows that the true values, figure on the middle shows the prediction values computed by PMNN and figure on the right shows if the absolute error. As we can see, the first two figures are almost the same as each other and the absolute error in the last figure is so small that it shows PMNN perfectly learns the eigenfunction. To validate the performance of our method, we also test our method in higher dimensions in Table

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Table 1
Parameter settings of training PMNN for different dimensions.

| Methods | d  | N   | N_{epoch} | layers of MLP       |
|---------|----|-----|------------|---------------------|
| PMNN    | 1  | 10000 | 50000     | [1, 20, 20, 20, 20, 1] |
| PMNN    | 2  | 20000 | 50000     | [2, 20, 20, 20, 20, 1] |
| PMNN    | 5  | 50000 | 50000     | [5, 40, 40, 40, 40, 1] |
| PMNN    | 10 | 100000 | 100000   | [10, 80, 80, 80, 80, 1] |

Table 2
Errors of PMNN for different dimensions.

| Methods | d  | Exact λ | Approximate λ | Absolute Error | Relative Error |
|---------|----|---------|---------------|----------------|----------------|
| PMNN    | 1  | 90.1304 | 90.1302       | 2.2287E-04     | 2.4727E-06     |
| PMNN    | 2  | 80.2608 | 80.2603       | 4.9152E-04     | 6.1240E-06     |
| PMNN    | 5  | 50.6520 | 50.6513       | 6.7184E-05     | 1.3264E-05     |
| PMNN    | 10 | 1.3040  | 1.3004        | 3.5808E-03     | 2.7461E-03     |

2. There are 4 examples with different dimensions. The first two rows are the results of low dimensional equations which show that the approximate λ is close to exact λ and the absolute error and the relative error is small enough to demonstrate the accuracy of PMNN. The last two rows are results of higher dimensional equations with d = 5, 10 which also have good accuracy.

Figure 2: The eigenfunction of one dimensional equation compared with the exact eigenfunction shows that PMNN perfectly learns the eigenfunction.

4.2. Two Examples of Smallest Eigenvalue Problem

4.2.1. First Example of Smallest Eigenvalue Problem

To validate the performance of IPMNN, we solve the following problem in Ω = [0, 1]^d,

\[
\begin{align*}
-\Delta u &= \lambda u, \quad \text{in } \Omega, \\
 u &= 0, \quad \text{on } \partial \Omega.
\end{align*}
\]

The exact eigenvalues are given by \( \lambda = \pi^2 \sum_{i=1}^{d} k_i^2 \) and the eigenfunctions are \( \Pi_{i=1}^{d} \sin(k_i \pi x_i) \) with \( k_i = 1, 2, 3, \ldots \). Therefore, the smallest eigenvalue is given by \( \lambda = d \pi^2 \) and the associated eigenfunction is \( u = \Pi_{i=1}^{d} \sin(\pi x_i) \) where \( x_i \) is the i-th component of \( x \).
Table 3
Parameter settings of training IPMNN for the first example with different dimensions.

| Methods | $d$ | $N$  | $N_{\text{epoch}}$ | layers of MLP |
|---------|-----|------|-------------------|---------------|
| IPMNN   | 1   | 10000| 50000            | [1, 20, 20, 20, 20, 1] |
| IPMNN   | 2   | 20000| 50000            | [2, 20, 20, 20, 20, 1] |
| IPMNN   | 5   | 50000| 50000            | [5, 40, 40, 40, 40, 1] |
| IPMNN   | 10  | 100000| 100000            | [10, 80, 80, 80, 80, 1] |

Table 4
Errors of IPMNN for the first example with different dimensions.

| Methods   | $d$ | Exact $\lambda$ | Approximate $\lambda$ | Absolute Error | Relative Error |
|-----------|-----|-----------------|-----------------------|----------------|----------------|
| IPMNN     | 1   | 9.8696          | 9.8695                | 7.5631E-05     | 7.6630E-06     |
| Deep Ritz [1] | 1   | 9.8696          | 9.85                 | -              | 2.0E-03        |
| IPMNN     | 2   | 19.7392         | 19.7395              | 2.6073E-04     | 1.3209E-05     |
| IPMNN     | 5   | 49.3480         | 49.3485              | 4.8492E-04     | 9.8266E-06     |
| Deep Ritz [1] | 5   | 49.3480         | 49.29                | -              | 1.1E-03        |
| IPMNN     | 10  | 98.6960         | 98.6953              | 7.8492E-04     | 7.9529E-06     |
| Deep Ritz [1] | 10  | 98.6960         | 92.35               | -              | 6.43E-02       |

The same as the results of PMNN, Table 3 summarizes the parameters employed to train IPMNN for the first example with different dimensions. In addition, Figure 4 and Figure 5 show the difference of the exact eigenfunction and eigenfunction learned by IPMNN for the first example of one dimensional equation and two dimensional equation. Finally, Table 4 shows the results of the first example with different dimensions and the results are compared with Deep Ritz method [1]. All of them show IPMNN can accurately learn the smallest eigenvalue and the corresponding eigenfunction in low dimensions and high dimensions.

4.2.2. Fokker-Planck Equation

In this subsection we consider the linear Fokker-Planck equation with the periodic boundary conditions in $\Omega = [0, 2\pi]^d$

$$ - \Delta u - \nabla V \cdot \nabla u - \Delta V u = \lambda u, \quad \text{in} \quad \Omega, $$

(22)

where $V(x)$ is a potential function. The smallest eigenvalue is $\lambda = 0$ and the corresponding eigenfunction is $u(x) = e^{-V(x)}$, which can be used to compute the error. We consider an example $V(x) = \sin(\sum_{i=1}^{d} c_i \cos(x_i))$, where $c_i$ takes values in $[0.1, 1]$. This example is special for IPMNN. The original method can not directly solve for eigenvalue $\lambda = 0$, because it is not possible to get $A^{-1}$ which does not exist when the smallest eigenvalue $\lambda = 0$. However, SIPMNN is suitable for this problem, because we transform the smallest eigenvalue to a new one $\lambda' \neq 0$. 

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Figure 4: The eigenfunction of one dimensional equation for the first example compared with the exact eigenfunction shows that IPMNN perfectly learns the eigenfunction.

Figure 5: Heat maps with 3 figures show the eigenfunction of two dimensional equation for the first example. Figure on the left shows that the true values, figure on the middle shows the prediction values computed by IPMNN and figure on the right shows that the absolute error.

The same as before, Table 5 summarizes the parameters used to train SIPMNN for the first example with different dimensions. However, it is worth noting that the number of the first layer of the neural network is not the same as the number of dimensions \( d \). To enforce the periodic boundary conditions as discussed above, we need to change the number of neurons as \( 2dk \). In addition, Figure 6 and Figure 7 show the difference of the exact eigenfunction and eigenfunction learned by SIPMNN for the first example with one dimensional equation and two dimensional equation. Finally, Table 6 shows the results of the first example of different dimensions and the results are compared with FBSDE [17]. All of them show SIPMNN can accurately learn the smallest eigenvalue and the corresponding eigenfunction in low dimensions and high dimensions.

5. Conclusions

In this work, we propose three new methods PMNN, IPMNN and SIPMNN combined with power method, inverse power method and shifted inverse power method to solve high-dimensional eigenvalue problems with the dominant eigenvalue, the smallest eigenvalue and the smallest zero eigenvalue, respectively. In similar spirits of traditional methods, our methods focus on linear differential operators, enforce the boundary conditions and iteratively approximate the real eigenvalue and eigenfunction. However, compared with traditional methods, our methods have some differences
Table 5
Parameter settings of training SIPMNN for Fokker-Planck equation with different dimensions.

| Methods   | $d$ | $\alpha$ | $k$ | $N$  | $N_{\text{epoch}}$ | layers of MLP |
|-----------|-----|-----------|-----|------|---------------------|---------------|
| SIPMNN 1  | 1   | 1         | 3   | 10000| 50000               | [6, 20, 20, 20, 20, 1] |
| SIPMNN 2  | 2   | 1         | 3   | 20000| 50000               | [12, 40, 40, 40, 40, 1] |
| SIPMNN 5  | 5   | 1         | 3   | 50000| 50000               | [30, 60, 60, 60, 60, 1] |
| SIPMNN 10 | 10  | 1         | 3   | 100000| 100000          | [60, 80, 80, 80, 80, 1] |

Table 6
Errors of SIPMNN for Fokker-Planck equation with different dimensions.

| Methods   | $d$ | Exact $\lambda$ | Approximate $\lambda$ |
|-----------|-----|-----------------|------------------------|
| SIPMNN 1  | 1   | 1.5497E-06      |                        |
| SIPMNN 2  | 2   | 4.4227E-05      |                        |
| SIPMNN 5  | 5   | 3.2902E-05      |                        |
| FBSDE [17]| 5   | 3.08E-03        |                        |
| SIPMNN 10 | 10  | 1.0347E-04      |                        |
| FBSDE [17]| 10  | 3.58E-03        |                        |

Figure 6: The eigenfunction of one dimensional equation for Fokker-Planck equation compared with the exact eigenfunction shows that SIPMNN perfectly learns the eigenfunction.

with them. Specifically, instead of discretizing the differential operator to a matrix, we use AD to represent it. Then the conventional methods discretize the eigenfunction to one eigenvector, but our methods use the neural network to learn the eigenfunction. Although our methods also use eigenvector to represent the eigenfunction, it just is used in the training stage. Another difference is the iterations which is implemented by optimizing specially defined loss function.

Numerical experiments are carried out to evaluate the applicability and accuracy of the three proposed methods for high-dimensional eigenvalue problems. We compare the predicted eigenfunctions with the exact one for one and two dimensional problems. Both of them demonstrate that our methods can accurately learn the corresponding eigenfunction. Additionally, we show the eigenvalues for one, two, five and ten dimensional problems. Then the eigenvalue is compared with the true one and other proposed methods, like deep Ritz method or FBSDE. Again, better results are obtained.

Although good results are shown in the above section, there also are some important problems of efficiently using our methods to solve eigenvalue problems and they will be our future work. At first, we only concentrate on linear
differential operators and self-adjoint operators in this work. Therefore, we may need to find new methods or augment the proposed methods now to solve for some other operators. In addition, the enforcement of boundary conditions is necessary for the methods. If it is enforced by the same way of PINN, it may be difficult to train the neural network. Furthermore, the dominant eigenvalue and the smallest eigenvalue is not multiple which means that if the eigenvalue we want to solve for follows the order like $|\lambda_1| \leq (\geq) |\lambda_2|$ and there exists two eigenvalues $\lambda_i = |\lambda_1|$, $\lambda_j = -|\lambda_1|$, our methods will get confused about this condition. Finally, the sampling algorithm and the number of sampling points are also important for our methods. Therefore, exploring how can they affect the accuracy will be one future work too.

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