Solving high-dimensional eigenvalue problems using deep neural networks: A diffusion Monte Carlo like approach

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Abstract

We propose a new method to solve eigenvalue problems for linear and semilinear second order differential operators in high dimensions based on deep neural networks. The eigenvalue problem is reformulated as a fixed point problem of the semigroup flow induced by the operator, whose solution can be represented by Feynman-Kac formula in terms of forward-backward stochastic differential equations. The method shares a similar spirit with diffusion Monte Carlo but augments a direct approximation to the eigenfunction through neural-network ansatz. The criterion of fixed point provides a natural loss function to search for parameters via optimization. Our approach is able to provide accurate eigenvalue and eigenfunction approximations in several numerical examples, including Fokker-Planck operator, linear and nonlinear Schrödinger operators in high dimensions.

1 Introduction

Many fundamental problems in scientific computing can be reduced to the computation of eigenvalues and eigenfunctions of an operator. One primary example is the electronic structure calculations, namely, computing the leading eigenvalue and eigenfunction of the Schrödinger operator. If the dimension of the state variable is low, one can use classical approaches, such as the finite difference method or spectral method, to discretize the operator and to solve the eigenvalue problem. However, these conventional, deterministic approaches suffer from the so-called curse of dimensionality, when the underlying dimension becomes high, since the degree of freedom grows exponentially as the dimension increases.

For high-dimensional problems, commonly arising from quantum mechanics, statistical mechanics, and finance applications, stochastic methods become more attractive and in many situations the only viable option. In the context of quantum mechanics, two widely used approaches for high-dimensional eigenvalue problems are the variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC) methods [1, 2, 3, 4, 5, 6]. These two approaches deal with the high dimensionality via different strategies. VMC relies on leveraging chemical knowledge to propose an ansatz of eigenfunction (wavefunction in the context of quantum mechanics) with parameters to be optimized under the variational formulation of the eigenvalue problem. The Monte Carlo approach is used to approximate the gradient of the energy with respect
to the parameters at each optimization iteration step. On the other hand, DMC represents the density of the eigenfunction with a collection of particles which follows the imaginary time evolution given by the Schrödinger operator, via a Feynman-Kac representation of the semigroup. It can be understood as a generalization of the classical power method from finite-dimensional matrices to infinite-dimensional operators. In electronic structure calculations, DMC usually can give more accurate eigenvalues compared with VMC, which relies on the quality of the proposed ansatz, while the particle representation of DMC often falls short to provide other information of the eigenfunction, such as its derivatives, unlike VMC.

As discussed above, one key to solving high-dimensional eigenvalue problems is the choice of function approximation to the targeted eigenfunction, ranging from the grid-based basis, spectral basis, to nonlinear parametrizations used in VMC, and to particle representations in DMC. Given the recent compelling success of neural networks in representing high-dimensional functions with remarkable accuracy and efficiency in various computational disciplines, it is fairly attempting to introduce neural networks to solve high-dimensional eigenvalue problems. This idea has been recently investigated under the variational formulation by [7, 8, 9, 10, 11, 12]. Particularly [9, 10, 11, 12] has shown the exciting potential of solving the many-electron Schrödinger equation with neural networks within the framework of VMC. On the other hand, how to apply neural networks in the formalism of DMC has not been explored in the literature, which leaves a natural open direction to investigate.

In this paper, we propose a new algorithm to solve high-dimensional eigenvalue problem for the second-order differential operators, in a similar spirit of DMC while based on the neural network parametrization of the eigenfunction. The eigenvalue problem is reformulated as a parabolic equation, whose solution can be represented by (nonlinear) Feynman-Kac formula in terms of forward-backward stochastic differential equations. Then we leverage the recently proposed deep BSDE method [13, 14] to seek optimal eigenpairs. Specifically, two deep neural networks are constructed to represent the eigenfunction and its scaled gradient. Then the neural network is propagated according to the semigroup generated by the operator. The loss function is defined as the difference between the neural networks before and after the propagation. Compared to conventional DMC, the proposed algorithm provides a direct approximation to the target eigenfunction, which overcomes the shortcoming in providing the gradient information. Moreover, since the BSDE formulation is valid for nonlinear operators, our approach can be extended to high-dimensional nonlinear eigenvalue problems, also validated in our numerical examples.

The rest of this paper is organized as follows. In Section 2, we introduce the algorithm to solve the eigenvalue problem. In Section 3, numerical examples are presented. We conclude in Section 4 with an outlook for future work.

2 Numerical methods

2.1 Method for linear operator

We consider the eigenvalue problem

$$\mathcal{L}\psi = \lambda\psi,$$

on $\Omega = [0, 2\pi]^d$ with periodic boundary condition where $\mathcal{L}$ is a linear operator of the form

$$\mathcal{L}\psi(x) = -\frac{1}{2} \text{Tr} \left( \sigma(x)\sigma^\top(x) \text{Hess}(\psi)(x) \right) - b(x) \cdot \nabla \psi(x) + f(x)\psi(x).$$
\(\sigma(x)\) is a \(d \times d\) matrix function such that \(\sigma(x)\sigma^\top(x)\) is uniformly elliptic, \(\nabla \psi\) denotes the gradient of \(\psi\), \(b(x)\) is a \(d\)-dimensional vector field and \(\text{Hess}(\psi)\) denotes the Hessian matrix of \(\psi\).

To solve this eigenvalue problem, we augment a time variable and consider the following backward parabolic partial differential equation (PDE) in the time interval \([0, T]\):

\[
\begin{aligned}
\partial_t u(t,x) - \mathcal{L}u(t,x) + \lambda u(t,x) &= 0 \quad \text{in } [0, T] \times \Omega, \\
u(T,x) &= \Psi(x) \quad \text{on } \Omega.
\end{aligned}
\]  

(3)

This is essentially a continuous time analog of the power method for matrix eigenvalue problem. Let us denote the solution of (3) as \(u(T - t, \cdot) = \mathcal{P}_T^\lambda \Psi\) (note that the backward propagator \(\{\mathcal{P}_t^\lambda\}_{t \leq T}\) forms a semigroup, i.e., \(\mathcal{P}^\lambda_{t_1} \circ \mathcal{P}^\lambda_{t_2} = \mathcal{P}^\lambda_{t_1+t_2}\)). According to the spectral theory of the elliptic operator, if \(\Psi\) is a stationary solution of (3), i.e., \(\mathcal{P}_T^\lambda \Psi = \Psi\), then \((\lambda, \Psi)\) must be an eigenpair of \(\mathcal{L}\). Therefore, we can minimize the “loss function” \(\|\mathcal{P}_T^\lambda \Psi - \Psi\|^2\) with respect to \((\lambda, \Psi)\) to solve the eigenvalue problem. While this is a non-convex optimization problem, we expect local convergence to a valid eigenpair with appropriate initialization.

The reformulation above turns the eigenvalue problem into solving a parabolic PDE in high dimensions. For the latter, we can leverage the recently developed deep BSDE method [13, 14, 15] (which is why the parabolic PDE (3) is written backward in time). Let \(X_t\) solve the stochastic differential equation (SDE)

\[dX_t = \sigma(X_t) \, dW_t,\]  

(4)

or in the integral form

\[X_t = X_0 + \int_0^t \sigma(X_s) \, dW_s,\]  

(5)

where \(W_t\) is a \(d\)-dimensional Brownian motion, and \(X_0\) is sampled from some initial distribution \(\nu\). Then according to Itô’s formula, the solution to (3), \(u(t, x)\) satisfies

\[u(t, X_t) = u(0, X_0) + \int_0^t (f(X_s)u(s, X_s) - \lambda u(s, X_s) - b(X_s)\nabla u(s, X_s)) \, ds + \int_0^t \sigma(X_s)^\top \nabla u(s, X_s) \, dW_s.\]  

(6)

Note that simulating the two SDEs (5) and (6) is relatively simple even in high dimensions, while directly solving the PDE (3) is intractable. We remark that it is possible to add a drift term \(b(X_t) \, dt\) to the SDE (4) and modify (6) accordingly (see the discussion below).

Of course, a priori in (6) for both \(u(s, \cdot)\) and \(\nabla u(s, \cdot)\) are unknown, while we know that if we set \(u(s, \cdot) = \Psi(\cdot)\), the eigenfunction we look for, and \(\nabla u(s, \cdot) = \nabla \Psi(\cdot)\), the solution \(u(t, \cdot)\) remains \(\Psi(\cdot)\) for all \(t\). The idea of our method is then to use two neural networks, \(\mathcal{N}_\Psi\) and \(\mathcal{N}_{\sigma^\top \nabla \Psi}\) as ansatz for the eigenfunction \(\Psi\) and its scaled gradient \(\sigma^\top \nabla \Psi\), respectively. Assigning \(u(0, X_0) = \mathcal{N}_\Psi(X_0)\) and \(\sigma(X_s)^\top \nabla u(s, X_s) = \mathcal{N}_{\sigma^\top \nabla \Psi}(X_s)\) in (6), the discrepancy for the propagated solution, i.e.,

\[
\mathbb{E}_{X_0 \sim \nu} \left[ \eta_1 |\mathcal{N}_\Psi(X_T) - u(T, X_T)|^2 + \eta_2 |\mathcal{N}_{\sigma^\top \nabla \Psi}(X_T) - \sigma^\top(X_T) \nabla \mathcal{N}_\Psi(X_T)|^2 \right]
\]  

(7)

then indicates the accuracy of the approximation. Here, we use \(|\cdot|\) to denote the absolute value of a number or the Euclidean norm of a vector according to the context. Note that the second term above penalizes the discrepancy between the approximation of \(\Psi\) and its gradient, where \(\eta_1, \eta_2\) are two weight hyperparameters. Therefore, using the above discrepancy as a loss function to optimize the triple \((\lambda, \mathcal{N}_\Psi, \mathcal{N}_{\sigma^\top \nabla \Psi})\) gives us a
scheme to solve the eigenvalue problem. The above procedure can be directly extended to semilinear case
where \( f \) depends on \( \Psi \) and \( \nabla \Psi \), as we will discuss in Section 2.3.

To employ the above framework in practice, we numerically discretize the SDEs (5) and (6) using
Euler–Maruyama method with a given partition of interval \([0, T] : 0 = t_0 < t_1 < \cdots < t_N = T:\)
\[
X_0 = X_0, \quad X_{n+1} = X_n + \sigma(X_n) \Delta W_n \tag{8}
\]
and
\[
U_0 = \nabla \Psi(X_0), \quad U_{n+1} = U_n + \left( \int \sigma(X_n) \Delta t_n + \nabla \sigma \nabla \Psi(X_n) \Delta W_n, \tag{9}
\]
for \( n = 0, 1, \ldots, N - 1 \). Here \( \Delta t_n = t_{n+1} - t_n, \Delta W_n = W_{n+1} - W_n \), and we use \( X_t \) and \( U_t \) to
represent the continuous and discretized stochastic process, respectively. The noise terms \( \Delta W_n \) have the
same realization in (8) and (9), as in the forward-backward SDEs (5) and (6).

The loss function (7) then corresponds to the discrete counterpart:
\[
\mathbb{E}_{X_0 \sim \nu} \left[ \eta_1 \left| \nabla \Psi(X_T) - U_T \right|^2 + \eta_2 \left| \nabla \sigma \nabla \Psi(X_T) - \sigma^\top(X_T) \nabla \Psi(X_T) \right|^2 \right], \tag{10}
\]
where \( \nabla \Psi \) is the gradient of neural network \( \Psi \) with respect to its input. In practice, the expectation
in (10) is further approximated by Monte Carlo sampling, which is similar to the empirical loss often used
in the supervised learning context. For a given batch size \( K \), we sample \( K \) points \( \{X_0^k\}_{k=1}^K \) of the initial
state from the distribution \( \nu \) at each training step and estimate the gradient of the loss with respect to the
trainable parameters using the empirical Monte Carlo average of (10):
\[
\frac{1}{K} \sum_{k=1}^K \left[ \eta_1 \left| \nabla \Psi(X_T^k) - U_T^k \right|^2 + \eta_2 \left| \nabla \sigma \nabla \Psi(X_T^k) - \sigma^\top(X_T^k) \nabla \Psi(X_T^k) \right|^2 \right]. \tag{11}
\]
We remark that the definition of dynamics (5) is not unique and implicitly affects the detailed computation
of the loss function (10) and (11). Specifically, in (5), the diffusion term \( \sigma(x) \) is determined by the operator
(2) while the choice of initial distribution and the drift term has some flexibility. If the drift in (5) changes,
one can change the associated drift in (6) according to Itô’s formula and define the loss again as (10)
and (11). In this work, we choose the form of (5) without the drift and \( \nu \) being the uniform distribution
on \( \Omega \) to ensure that the whole region is reasonably sampled for the optimization of eigenfunction. Some
importance sampling can be also used if some prior knowledge of the eigenfunction is available, which we
will not go into further details in this work.

At a high level, our algorithm is in a similar vein as the power method for solving the eigenvalue
problem in linear algebra. Both algorithms seek for solutions that are stationary under the propagation.
However, one distinction is that our algorithm is not only for solving the first eigenvalue, but rather
general eigenvalue, mainly depending on the initialization of \( \lambda \). On the other hand, we find in numerical
experiments that if \( \lambda \) is initialized small enough, it will always converge to the first eigenvalue.

In practice, we use fully-connected feed-forward neural networks for the approximation of \( \Psi \) and \( \sigma^\top \nabla \Psi \),
respectively. To ensure periodicity of the neural network outputs, the input vector \( x = (x_1, \ldots, x_d) \) is first
mapped into a fixed trigonometric basis \( \{ \sin(jx_i), \cos(jx_i) \}_{i=1, j=1}^d M \) of order \( M \). Then the vector consisting
of all basis components are fed into fully-connected neural networks with some hidden layers, each with
several nodes. See Figure 1 for illustration of the involved network structure. We use ReLU as the activation
function and optimize the parameters with the Adam optimizer [16].
2.2 Normalization

The above loss has one caveat though, as the trivial solution ($\mathfrak{N}_\Psi = 0, \mathfrak{N}_{\sigma^\top \nabla \Psi} = 0$) is a global minimizer. Therefore, normalization is required to exclude such a trivial case. We seek for eigenfunctions $\Psi$ such that
\[
\int_{\Omega} \Psi^2 = |\Omega|, \text{ i.e., } \frac{1}{|\Omega|} \|\Psi\|_{L^2}^2 = 1.
\]
To proceed, we define the normalization constant
\[
Z_\Psi = \text{sign} \left( \int_{\Omega} \mathfrak{N}_\Psi(x) \, dx \right) \left( \frac{1}{|\Omega|} \int_{\Omega} \mathfrak{N}_\Psi(x)^2 \, dx \right)^{1/2}.
\]
Thus dividing $\mathfrak{N}_\Psi$ by $Z_\Psi$, we enforce that the parametrized function ensures the normalization condition. Note that the first term on the right hand side of (12) is introduced to fix the global sign ambiguity of the eigenfunction.

In computation, given the parameters of $\mathfrak{N}_\Psi$, we do not have direct access to $Z_\Psi$. Instead, at the $\ell$-th step of training, we use our batch of $K$ data samples to approximate $Z_\Psi$ via
\[
\hat{Z}_\Psi^\ell = \text{sign} \left( \sum_{k=1}^{K} \mathfrak{N}_\Psi(\mathcal{X}_0^k, \ell) \right) \left( \frac{1}{K} \sum_{k=1}^{K} \mathfrak{N}_\Psi(\mathcal{X}_0^k, \ell)^2 \right)^{1/2},
\]
where the superscripts in $\mathcal{X}_0^k, \ell$ serves as the index of batch ($k$) and index of the training step ($\ell$). The above is a Monte Carlo estimation of (12) if $\mathcal{X}_0$ is sampled from uniform distribution (which we assume in this work). Due to the normalization procedure, $\hat{Z}_\Psi^\ell$ will enter into the loss function, and thus the stochastic gradient based on the empirical average over the batch becomes biased (since $\mathbb{E}(A/B) \neq \mathbb{E}A/\mathbb{E}B$ in general).

To reduce the bias and make the training more stable, we introduce an exponential moving average scheme

\footnote{The reason we set $\frac{1}{|\Omega|} \|\Psi\|_{L^2}^2 = 1$ instead of $\|\Psi\|_{L^2}^2 = 1$ is because we want to consider the problem in high dimensions in the domain $\Omega = [0, 2\pi]^d$. Consider the trivial case when $\mathcal{L} = -\Delta$, whose smallest eigenvalue is $\lambda = 0$ and any constant function is a corresponding eigenfunction. If $\|\Psi\|_{L^2}^2 = 1$, the constant function becomes $\Psi = (\frac{1}{\sqrt{d}})^d$, which vanishes as $d \to \infty$; instead the normalization $\|\Psi\|_{L^2}^2 = |\Omega|$ keeps the pointwise-value of $\Psi$ as order 1, which benefits the training process.}
to the normalization constant in order to reduce the dependence of the loss to the estimated normalization constant of the current batch. In our implementation, we use
\[ Z^\ell_q = \gamma_{\ell} Z^{\ell-1}_q + (1 - \gamma_{\ell}) Z^\ell_q. \]  
Here \( \gamma_{\ell} \in (0, 1) \) is the moving average coefficient for decay. It is observed that small \( \gamma_{\ell} \) at the beginning makes training efficient, and later on its value is increased such that the gradient is less biased.

Given the introduced normalization factor, the neural network approximation \( \mathcal{U}_0 \) in the updating scheme (9) is replaced by (we suppress the training step index in \( X \))
\[ \mathcal{U}_0^k = \frac{\mathcal{N}_\psi(X_0^k)}{Z^\ell_q}, \]
and we would hope to reduce the discrepancy between the solution of (9) at time \( T \) and the normalized neural network approximation \( \mathcal{N}_\psi(X_0^k)/Z^\ell_q \) through training. The associated batch approximation of loss function used for the computation of stochastic gradient is as follows
\[ \frac{1}{K} \sum_{k=1}^{K} \left( \eta_1 \left| \frac{\mathcal{N}_\psi(X_T^k)}{Z^\ell_q} - \mathcal{U}_0^k \right|^2 + \eta_2 \left| \mathcal{N}_{\sigma^T \nabla \psi}(X_T^k) - \frac{\sigma^T(X_T^k) \nabla \mathcal{N}_\psi(X_T^k)}{Z^\ell_q} \right|^2 \right) + \eta_3 (Z_0 - Z^\ell_q)^+. \]  
In the last term above \( Z_0 \) is a hyperparameter and \( \eta_3 \) is the associated weight. This term is introduce to prevent \( Z^\ell_q \) being too small; otherwise the normalization would become unstable. In each training step, we calculate the gradient of (16) with respect to all parameters to be optimized, including the eigenvalue \( \lambda \) and parameters in the neural network ansatz \( \mathcal{N}_\psi \) and \( \mathcal{N}_{\sigma^T \nabla \psi} \). Note that in (16) we do not normalize \( \mathcal{N}_{\sigma^T \nabla \psi} \) since its scale has been determined implicitly. When \( K \) is reasonably large and if we neglect the discretization error of simulating the SDEs, the empirical sum in (16) can be interpreted as a Monte Carlo approximation to the loss (ignoring the sign ambiguity)
\[ \mathbb{E}_{X_0 \sim \nu} \left[ \eta_1 \left| \frac{\mathcal{N}_\psi(X_T)}{||\mathcal{N}_\psi||_2/||\Omega||^\frac{1}{2}} - u(T, X_T) \right|^2 + \eta_2 \left| \mathcal{N}_{\sigma^T \nabla \psi}(X_T) - \frac{\sigma^T(X_T) \nabla \mathcal{N}_\psi(X_T)}{||\mathcal{N}_\psi||_2/||\Omega||^\frac{1}{2}} \right|^2 \right], \]
where \( u(T, X_T) \) is defined as (6) except that \( u(0, X_0) = ||\Omega||^\frac{1}{2} \mathcal{N}_\psi(X_0)/||\mathcal{N}_\psi||_2 \). We remark that the normalization procedure introduced here shares a similar spirit with Batch Normalization [17], which is widely used in the training of neural networks.

We summarize our algorithm as pseudocode in Algorithm 1.

2.3 Method for semilinear operator

Our algorithm can be generalized to solve eigenvalue problems for semilinear operator
\[ \mathcal{L}\psi(x) = \frac{1}{2} \text{Tr} \left( \sigma(x) \sigma^T(x) \text{Hess}(\psi)(x) \right) - b(x) \cdot \nabla \psi(x) + f(x, \psi(x), \sigma^T(x) \nabla \psi(x)). \]

The method for semilinear problems is almost the same to previous sections, except for a few modifications. The SDE for \( X_t \) is the same as (5) while equation (6) that the solution of the PDE (3) satisfies becomes
\[ u(t, X_t) = u(0, X_0) + \int_0^t \left( f(X_s, u(s, X_s), \sigma^T(X_s) \nabla u(s, X_s)) - b(X_s) \nabla u(s, X_s) - \lambda u(s, X_s) \right) \, ds + \int_0^t (\nabla u(s, X_s))^\top \sigma(X_s) \, dW_s. \]
Algorithm 1 Neural network based eigensolver

Input: operator $L$, terminal time $T$, number of time intervals $N$, loss weights $\eta_1, \eta_2, \eta_3$, $Z_0$, neural network structures, number of iterations, learning rate, batch size $K$, moving average coefficient $\gamma$ in (14)

Output: eigenvalue $\lambda$, eigenfunction $\Psi$ and rescaled gradient $\sigma^\top \nabla \Psi$

initialization: eigenvalue $\lambda$, $\Psi$, $\sigma^\top \nabla \Psi$ and normalization factor $Z_0$

for $\ell = 1$ to the number of iterations do
  sample $K$ points of $X_0$ and sample $K$ Wiener processes $W_t$
  compute $X_{tn}$ via (8)
  compute the normalization factor $Z_\ell \Psi$ via (13) and (14)
  normalize and propagate via (15) and (9)
  compute the gradient of loss (16) with respect to the trainable parameters
  update the trainable parameters by Adam method
end for

The discretization of $X_t$, equation (8), remains unchanged while equation (9) needs modification according to (19):

$$
\tilde{U}_{n+1} = U_n + \left( f(X_{tn}, U_{tn}, \sigma^\top \nabla \Psi) - \lambda U_n - (b \sigma^\top \sigma^\top \Psi)(X_{tn}) \right) \Delta t_n + \Psi^\top \nabla \Psi(X_{tn}) \Delta W_n,
$$

where Clip is a clipping function given by

$$
\text{Clip}(u, -Q, Q) = \begin{cases} 
  -Q, & \text{if } u < -Q; \\
  u, & \text{if } -Q \leq u \leq Q; \\
  Q, & \text{if } u > Q.
\end{cases}
$$

Here we introduce the clipping function to prevent numerical instability caused by the nonlinearity of $f$ in (19), especially at the early stage of training. It checks $U_n$ and replaces those whose absolute values are larger than $Q$ with $\text{sign}(U_n)Q$, where $Q > 0$ is an upper bound of the absolute value of the true normalized eigenfunction. Given the modified forward dynamics (20), the loss function for the semilinear operators are defined the same as (16), and the training algorithm is the same too.

3 Numerical results

In this section, we report the performance of the proposed eigensolver in three examples: the Fokker-Planck equation, the linear Schrödinger equation, and the nonlinear Schrödinger equation. The domain $\Omega$ is always $[0, 2\pi]^d$ with periodic boundary condition. In each example we consider the dimension $d = 5$ and $d = 10$. The hyperparameters are given in Appendix B. We examine the errors of the prescribed eigenvalue, the associated eigenfunction, and the gradient of the eigenfunction. The errors for eigenfunctions and gradients of eigenfunctions are computed in $L^2$ sense, approximated through a set of validation points. Given a set of validation points $\{X^k\}_{k=1}^K$, we use the quantity

$$
\text{err}_\Psi := \left[ \frac{1}{K} \sum_{k=1}^K \left( \frac{\Psi(X^k)}{Z^k_\Psi} - \left( \frac{\Psi(X^k)}{Z^k_\Psi} \right)^2 \right)^2 \right]^{1/2}
$$

(22)
to measure the error for eigenfunction where $Z^\ell_\Psi$ is computed via equation (14), with a known reference eigenfunction $\Psi$. We use

$$
er_{\sigma}^\top \nabla \Psi := \left[ \frac{1}{Kd} \sum_{k=1}^{K} \left| \frac{\sigma(X^k)}{\sum_{m=1}^{K} |\sigma(X^m)^\top \nabla \Psi(X^m)|^2} \right|^{\frac{1}{2}} \right]^{2^{\frac{1}{2}}} \right]^{2^{\frac{1}{2}}} (23)
$$

to quantify the error for the gradient approximation. We record and plot the error every 100 steps in the training process, with a smoothed moving average of window size 10. The final error reported is based on the average of last 1000 steps. Besides the errors above, we also visualize and compare the density of the true eigenfunction and its neural network approximation (since it is hard to visualize the high-dimensional eigenfunction directly). The density of a function $\Psi$ is defined as the probability density function of $\Psi(X)$ where $X$ is a uniformly distributed random variable on $\Omega$. In practice, the density is approximated by Monte Carlo sampling. As shown below, in all three examples, we find that the eigenpairs (with gradients) are solved accurately and the associated densities match well.

### 3.1 Fokker-Planck equation

In this subsection we consider the linear Fokker-Planck operator

$$
\mathcal{L} \psi = -\Delta \psi - \nabla \cdot (\psi \nabla V),
$$

where $V(x)$ is a potential function. The smallest eigenvalue of $\mathcal{L}$ is $\lambda_1 = 0$ and the corresponding eigenfunction is $\Psi(x) = e^{-V(x)}$, 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 $x_i$ is the $i$-th coordinate of $x$, and $c_i$ takes values in $[0,1]$. The function $V$ is periodic by construction. Figure 2 shows the density and error curves for the Fokker-Planck equation in $d = 5$ and $d = 10$. For $d = 5$, the final errors of the eigenvalue, eigenfunction, and the scaled gradient are $3.46e-3$, $2.406\%$, and $4.914\%$. For $d = 10$, the final errors are $3.67e-3$, $1.432\%$, and $4.701\%$.

### 3.2 Linear Schrödinger equation

In this subsection we consider the Schrödinger operator

$$
\mathcal{L} \psi = -\Delta \psi + V \psi,
$$

where $V(x)$ is a potential function. Here we choose $V(x) = \sum_{i=1}^{d} c_i \cos(x_i)$, in which $c_i$ takes values in $[0,0.2]$. With potential function being such a form, the problem is essentially decoupled. Therefore we are able to compute the eigenvalues and eigenfunctions in each dimension through the spectral method and obtain the final first eigenpair with high accuracy for comparison. The computation details are provided in Appendix A. Figure 3 shows the density and error curves for the Schrödinger equation in $d = 5$ and $d = 10$. For $d = 5$, the final errors of the eigenvalue, eigenfunction, and the scaled gradient are $3.46e-3$, $2.406\%$, and $4.914\%$. For $d = 10$, the final errors are $3.67e-3$, $1.432\%$, and $4.701\%$.

### 3.3 Nonlinear Schrödinger equation

We finally consider a nonlinear Schrödinger operator with a cubic term, arising from the Gross–Pitaevskii equation \cite{18, 19} for the single-particle wavefunction in a Bose-Einstein condensate:

$$
\mathcal{L} \psi = -\Delta \psi + \epsilon \psi^3 + V \psi.
$$

(24)
Here we assume $\epsilon = 1$ and consider a specific external potential

$$V(x) = -\frac{1}{c^2} \exp \left( \frac{2}{d} \sum_{i=1}^{d} \cos x_i \right) + \sum_{i=1}^{d} \left( \frac{\sin^2 x_i}{d^2} - \frac{\cos x_i}{d} \right) - 3,$$

such that $\lambda = -3, \Psi(x) = \exp(\ell \sum_{j=1}^{d} \cos(x_j))/c$ is an eigenpair of the operator (24). Here $c$ is a positive constant such that $\int_{\Omega} \Psi^2(x)dx = |\Omega|$. Figure 4 shows the density and error curves for the nonlinear Schrödinger equation in $d = 5$ and $d = 10$. For $d = 5$, the final errors of the eigenvalue, eigenfunction, and the scaled gradient are 1.53e-3, 0.807%, and 4.367%. For $d = 10$, the final errors are 2.6e-4, 0.460%, and 3.552%.

## 4 Conclusion and future works

In this paper, we propose a new method to solve eigenvalue problems in high dimensions using neural networks. Our method is able to compute both eigenvalues and corresponding eigenfunctions (with gradients) with high accuracy.
There are several natural directions for future work. First, to apply our methodology to quantum many-body systems, we need to respect the permutation symmetry in our ansatz for the wavefunctions. Previous works [9, 12, 11, 10] have proposed various flexible neural-network ansatz to incorporate in the symmetry, which can be combined with our approach. Moreover, in DMC, importance sampling techniques are often essential to improve the accuracy. In our context, this means to choose a better underlying diffusion process guided by a trial wavefunction depending on the problem. Last, the scalability of the method has to be tested on larger systems beyond the toy numerical examples in this work.

On the theoretical aspects, the understanding of the stability and convergence of the proposed method is a fascinating future direction. While the general analysis might be quite difficult given the highly nonlinear approximation induced by the neural networks and also the complicated optimization strategy, some perturbative analysis, especially in the linearized regime, might be possible. We will leave these to future works.

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Figure 4: Top: density of $\Psi(x)$ for nonlinear Schrödinger equation with $d = 5$ (left) and $d = 10$ (right). Bottom: associated error curves in the training process with $d = 5$ (left) and $d = 10$ (right).

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Appendices

A Spectrum method for linear Schrödinger equation

Suppose that the potential function in the linear Schrödinger operator \( L = -\Delta + V \) is decoupled with the form \( V(x) = \sum_{j=1}^{d} c_j \cos(x_j) \), then we can solve the corresponding eigenvalue problem in a decoupled way. Specifically, assume we can solve the one-dimensional eigenvalue problem

\[
-\Psi''_j(x) + c_j \cos(x) \Psi_j(x) = \lambda_j \Psi_j(x), \quad x \in [0, 2\pi].
\]  

(26)

Then one can easily verify that \( \lambda = \sum_{j=1}^{d} \lambda_j \) and

\[
\Psi(x) = \prod_{j=1}^{d} \Psi_j(x_j)
\]

(27)
together define an eigenpair of the original high-dimensional Schrödinger operator.

To solve (26), we can employ the classical spectrum method. For a fixed \( N \in \mathbb{N} \), assume that

\[
\Psi_j(x) = \sum_{m=-N}^{N} a_m^j e^{imx},
\]

(28)

then

\[
\Psi'_j(x) = \sum_{m=-N}^{N} ma_m^j e^{imx} i.
\]

(29)

Let \( \varphi_n(x) = e^{inx} \ (n = -N, \ldots, N) \) be the test functions. By (26) and periodicity, we have

\[
\int_{0}^{2\pi} (\Psi'_j(x)\varphi'_n(x) + c_j \cos(x) \Psi_j(x)\varphi_n(x))dx = \lambda_j \int_{0}^{2\pi} \Psi_j(x)\varphi_n(x)dx.
\]

(30)

Since \( \int_{0}^{2\pi} e^{inx} e^{inx} \ dx = 2\pi \delta_{m+n} \) and \( \int_{0}^{2\pi} \cos(x) e^{inx} e^{inx} \ dx = \frac{1}{2} \int_{0}^{2\pi} (e^{i(m+n+1)x} + e^{i(m+n-1)x})dx = \pi (\delta_{m+n+1} + \delta_{m+n-1}) \), the left- and right-hand sides of (30) become

\[
\begin{align*}
\int_{0}^{2\pi} (\Psi'_j(x)\varphi'_n(x) + c_j \cos(x) \Psi_j(x)\varphi_n(x))dx &= \sum_{m=-N}^{N} a_m^j \int_{0}^{2\pi} (-mne^{inx} + c_j \cos(x))e^{inx}dx \\
&= \sum_{m=-N}^{N} a_m^j \pi (-2mn\delta_{m+n} + c_j \delta_{m+n+1} + c_j \delta_{m+n-1}) \\
&= \pi (2n^2 a_{-n} + c_j a_{-n-1} + c_j a_{-n+1}),
\end{align*}
\]

(31)

(assuming \( a_m = 0 \) for \( |m| > N \)) and

\[
\int_{0}^{2\pi} \Psi_j(x)\varphi_n(x)dx = 2\pi a_{-n},
\]

(32)
respectively. Therefore, equation (30) can be rewritten in the matrix form:

\[
\pi \begin{bmatrix}
2N^2 & c_j & \cdots & \cdots & \cdots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
c_j & \cdots & \cdots & \cdots & 2N^2
\end{bmatrix}
\begin{bmatrix}
a_j \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
a_j \\
a_j \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
a_j \\
a_j \\
\vdots \\
a_{j-N} \\
a_j \\
a_j \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
a_j \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
\vdots \\
2N^2
\end{bmatrix}
= 2\pi \lambda_j
\begin{bmatrix}
a_j \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
a_j \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
a_j \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
a_j \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
\vdots \\
a_{j-N} \\
\vdots \\
2N^2
\end{bmatrix}
\] (33)

This is a standard eigenvalue problem in numerical algebra. Suppose \( \tilde{\lambda}_j \) and \((a_{-N}, \ldots, a_N)\) is the eigenvalue and associated eigenvector of the matrix in (33), then \( \lambda_j = \tilde{\lambda}_j/2 \) is the approximated eigenvalue in (26), and (28) provides the associated eigenfunction, which is equivalent to a real eigenfunction up to a complex constant.

B Hyperparameters in the numerical example

We first report hyperparameters commonly used in all three numerical examples and then list in Tables 1-3 those specific to the examples. In all three examples, the order of the trigonometric basis \( M = 5 \), the constant \( Z_0 = 2 \) for regularizing the normalization factor, the weight parameters in the loss \( \eta_1 = 1000, \eta_2 = 20, \eta_3 = 100 \). In the following tables, the structures of the neural networks are represented by vectors, whose elements denote the number of nodes within each layer. The learning rate and moving average decay \( \gamma_{\ell} \) are both piecewise constant, whose values and boundaries are given separately. For example, in 5-dimensional Fokker-Planck problem, the learning rate is \( 1e^{-4} \) for the first 30000 steps, \( 5e^{-5} \) from the 30001-st to the 60000-th step and \( 1e^{-5} \) after the 60000-th step. The moving average decay \( \gamma_{\ell} \) is defined similarly, with the same boundaries.

| Parameters                        | \( d = 5 \)       | \( d = 10 \)      |
|-----------------------------------|-------------------|-------------------|
| terminal time \( T \)             | 0.2               | 0.2               |
| number of time intervals \( N \)  | 80                | 120               |
| structure of neural networks      | [80, 80, 80]      | [300, 300, 300]   |
| number of iterations              | 80000             | 100000            |
| learning rate                     | \([1e^{-4}, 5e^{-5}, 1e^{-5}]\) | \([5e^{-5}, 2e^{-5}, 1e^{-5}]\) |
| moving average decay \( \gamma_{\ell} \) | \([0.2, 0.5, 0.9]\) | \([0.2, 0.5, 0.9]\) |
| piecewise constant boundaries      | \([30000, 60000]\) | \([60000, 80000]\) |
| batch size \( K \)                | 1024              | 1024              |

Table 1: Parameters for Fokker-Planck eigenvalue problems.
| Parameters                      | $d = 5$ | $d = 10$ |
|--------------------------------|---------|---------|
| terminal time $T$              | 0.3     | 0.3     |
| number of time intervals $N$   | 80      | 120     |
| structure of neural networks   | [80, 80, 80] | [300, 300, 300] |
| number of iterations           | 80000   | 80000   |
| learning rate                  | $[1e^{-4}, 5e^{-5}, 1e^{-5}]$ | $[5e^{-5}, 5e^{-5}, 1e^{-5}]$ |
| moving average decay $\gamma_\ell$ | [0.2, 0.5, 0.9] | [0.2, 0.5, 0.9] |
| piecewise constant boundaries  | [30000, 60000] | [40000, 60000] |
| batch size $K$                 | 1024    | 1024    |

Table 2: Parameters for linear Schrödinger eigenvalue problems.

| Parameters                      | $d = 5$ | $d = 10$ |
|--------------------------------|---------|---------|
| terminal time $T$              | 0.2     | 0.3     |
| number of time intervals $N$   | 120     | 200     |
| structure of neural networks   | [80, 80, 80] | [300, 300, 300] |
| number of iterations           | 60000   | 80000   |
| learning rate                  | $[5e^{-5}, 2e^{-5}, 1e^{-5}]$ | $[5e^{-5}, 2e^{-5}, 1e^{-5}]$ |
| moving average decay $\gamma_\ell$ | [0.2, 0.9, 0.99] | [0.1, 0.9, 0.99] |
| piecewise constant boundaries  | [20000, 40000] | [40000, 60000] |
| batch size $K$                 | 2048    | 2048    |

Table 3: Parameters for nonlinear Schrödinger eigenvalue problems.