Augmenting Basis Sets by Normalizing Flows

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Approximating functions by a linear span of truncated basis sets is a standard procedure for the numerical solution of differential and integral equations. Commonly used concepts of approximation methods are well-posed and convergent, by provable approximation orders. On the down side, however, these methods often suffer from the curse of dimensionality, which limits their approximation behavior, especially in situations of highly oscillatory target functions. Nonlinear approximation methods, such as neural networks, were shown to be very efficient in approximating high-dimensional functions. We investigate nonlinear approximation methods that are constructed by composing standard basis sets with normalizing flows. Such models yield richer approximation spaces while maintaining the density properties of the initial basis set, as we show. Simulations to approximate eigenfunctions of a perturbed quantum harmonic oscillator indicate convergence with respect to the size of the basis set.

1 Introduction

Numerical approximation schemes arise in many relevant problems that deal with solutions of (partial) differential and integral equations [1], where commonly used approximation methods rely on fix point iterations. Another popular class of approximation methods expands the sought target function by a linear span from a (countable) set of basis functions. In fact, when applied to the solution differential equations, this standard approach leads to spectral methods.

Spectral methods were studied quite extensively [2], where they enjoyed increasing popularity in various applications from computational science and engineering, especially for their good approximation properties. Despite their favorable approximation properties, their convergence rate degrades exponentially at increasing problem dimension. This phenomenon, referred to as the curse of dimensionality, is due to the linearity of the approximation method. This leads to severe limitations, e. g., in applications of quantum mechanics and dynamics, where the systems of interest are inherently high-dimensional and where approximations of large numbers of eigenfunctions to unbounded linear operators are required.

Nonlinear models, such as neural networks, have recently been explored as alternative approximation methods for solving (partial) differential equations [3]. Their efficiency in approximating high-dimensional functions for challenging applications, ranging from image recognition to natural language processing, shows their potential for solving high-dimensional differential equations, in particular for variational problems. One important problem class are infinite dimensional eigenvalue problems, e. g., Schrödinger equations, since they are strongly related to variational simulations of numerous physics phenomena and, moreover, they often demand solutions for a large number of eigenvalues.

Indeed, neural networks were successfully applied to various finite-[4] and infinite-dimensional [5] quantum systems, yielding higher accuracies at a lower computational scaling, in contrast to traditional methods. Using standard neural network architectures, such as multilayer perceptrons, however, reduces their reliability, due to the lack of analytic convergence results.

In addition, their concepts are widely restricted to modeling eigenfunctions corresponding to states with low energies.

In the physics applications that we have in mind, we are primarily interested in nonlinear approximation schemes, where standard basis sets are composed with normalizing flows [6], i. e., invertible parameterizable functions [1]. The aim of such a model is to increase the expressivity of standard basis sets, thereby enabling a more diverse and expansive approximation space. We restrict ourselves to the relevant case of basis sets of $L^2$. We show that augmented basis sets, i. e., standard $L^2$ basis sets composed with invertible parametrizable mappings, lead to a family of linear spaces that are all dense in $L^2$, whereby they generate much richer approximation spaces.

We use invertible residual neural networks [7] to augment the expressivity of Hermite functions, before we apply them to find the eigenfunctions of a perturbed quantum harmonic oscillator. Our results show fast convergence with respect to the size of the augmented basis. Moreover, we argue that the inductive bias attained by the use of an initial basis set allows for the
approximation of a larger number of eigenfunctions than what is possible with more flexible models, such as standard neural networks.

2 Augmenting Basis Sets

For an open domain $\Omega \subset \mathbb{R}^d$, let $L^2(\Omega)$ be the linear space of square integrable functions from $\Omega$ to $\mathbb{R}^d$. From now on, we drop the dependence on $\Omega$ for notational simplicity. Moreover, let $\{\phi_n\}_n$ denote a basis set of $L^2$ with inner product $\langle ., . \rangle$. Let $g_\theta : \Omega \rightarrow \Omega$ be a smooth parametrizable bijection. Finally, let $\phi$ denote the standard composition between functions.

Definition 2.1 (Augmented set of functions) On the above assumptions, we define an augmented set of functions $\{\phi_n^A\}_n$ by

$$\phi_n^A(x) := (g_n \circ g^{-1}_\theta)(x) |\det \nabla_x g^{-1}_\theta|^{1/2}.$$  

For simplicity, we drop the dependence of $g$ on $\theta$, and we define the weighted $L^2_{g^{-1}}$ space induced by the bijection $g$ as

$$L^2_{g^{-1}} := \left\{ f : \int |f|^2 |\det \nabla_x g^{-1}| dx < \infty \right\},$$

with the usual equivalence relation in $L^p$-spaces. We denote by $\langle ., . \rangle_{g^{-1}}$ the inner product on the weighted space $L^2_{g^{-1}}$, i.e.,

$$\langle f, h \rangle_{g^{-1}} = \int f(x) h(x) |\det \nabla_x g^{-1}| dx.$$

The following theorem shows that any augmented set of functions, as in Definition 2.1, is a basis set. This observation enables us to construct approximation spaces with good convergence properties.

Theorem 2.2 (Augmented basis sets) The augmented set of functions $\{\tilde{\phi}_n\}_n$ is an orthonormal basis of $L^2_{g^{-1}}$.

Proof. The orthonormality of the functions in $\{\tilde{\phi}_n\}_n$ can readily be seen by a simple change of variable. To prove that $\{\tilde{\phi}_n\}_n$ is a basis set for $L^2_{g^{-1}}$, we take one $f \in L^2_{g^{-1}}$ satisfying $f \perp \tilde{\phi}_n$ for all $n$. In this case, we have the orthogonality

$$0 = \langle \tilde{\phi}_n, f \rangle_{g^{-1}} = \int \phi_n(y) f(g(y)) dy \quad \text{for all } n.$$  

Since $\{\phi_n\}_n$ is a basis of $L^2$, we have $f \circ g \equiv 0$, which is equivalent to $\text{ran}(f \circ g) = \{0\}$. Given that $g^{-1}$ is invertible we have $\text{range}(g) = \text{domain}(g^{-1}) = \Omega$. Hence, $\text{range}(f \circ g) = \text{range}(f)$ and thus $f \equiv 0$. \hfill \Box

Note that $\{\tilde{\phi}_n\}_n$ being a basis of $L^2_{g^{-1}}$ is equivalent to $\{\phi_n^A\}_n$ being a basis of $L^2$. Also note that $\overline{\text{span}\{\phi_n^A\}}$ depends on $\theta$. In our numerical investigations, we work with the set of Hermite functions $\{\phi_n\}_n$. In one dimension these are defined by

$$\phi_n(x) := h_n(x) \exp(-x^2/2),$$  

where $h_n$ denotes the nth Hermite polynomial. Note that this set of functions is a basis of $L^2(\mathbb{R})$.

Now there are many ways to construct a parametrizable bijection $g$. As these bijections emerged in the machine learning community to perform generative modeling, the most common framework for constructing such bijections is via special types of neural networks. Here we use invertible residual networks [7] having the form $g(x) = x + k(x)$, where $k$ is a standard neural network with linear layers and nonlinear activations. It was shown that this model is invertible, if Lip($k$) < 1 [7], where Lip($k$) is the Lipschitz constant of $k$. To satisfy the invertibility condition for a residual network $k$, we employed Lipschitz-continuous nonlinear activation functions and divided the linear layer weight matrices by their spectral norm.

In the next section, we show how to numerically solve the Schrödinger equation for a perturbed quantum harmonic oscillator, in order to demonstrate the advantages of approximating $L^2$ functions with the augmented Hermite basis.

3 Numerical Investigation and Discussion

Let $\Omega := \mathbb{R}^d$. We consider approximating the eigenvalues of quantum mechanical Hamiltonian operators $H : D(H) \rightarrow L^2$, i.e., we aim at finding the eigenpairs $(E_k, \psi_k)$ that solve the Schrödinger equation

$$H \psi_k = E_k \psi_k, \quad \text{where } \int |\psi_k|^2 dx = 1 \quad \text{for } k = 0, 1, \ldots.$$  

To this end, we use a Bubnov-Galerkin numerical scheme [2]. We assume that $H$ is a self-adjoint operator, where we consider the generic case of $H = T + V$ with $T = -\frac{1}{2} \Delta$ denoting the kinetic-energy operator and $V$ denotes the scalar potential-energy.
following standard theories of quantum mechanics [8], we set $D(H) = \mathcal{H}^2$ for the Sobolev space of functions, which are square integrable along with their generalized partial derivatives up to second order.

We discretize problem (1) by using a truncated series of Hermite functions $\{\phi_n\}_{n=0}^{N-1}$ and a truncated series of augmented Hermite functions $\{\phi^A_n\}_{n=0}^{N-1}$, with the aim to compare the convergence properties of the two schemes as $N$ increases. Projecting (1) on the linear space of the two basis sets yields

$$\tilde{H} C_n = \tilde{E}_n C_n \quad \text{for } n = 0, \ldots, N - 1,$$

where $\tilde{H}$ is an $N \times N$ matrix whose $(i, j)$-th entry is $\tilde{H}[i, j] = \langle \phi_i, H \phi_j \rangle$ or $\langle \phi^A_i, H \phi^A_j \rangle$, for Hermite and augmented Hermite basis sets, respectively. Moreover, $C_n$ in (2) is a vector of size $N$. Hence, solving (1) boils down to solving the finite dimensional eigenvalue problem (2). Note that the approximation space in the case of using Hermite functions reads $V = \text{span}(\phi_0, \ldots, \phi_{N-1})$. In the case of augmented Hermite functions, the approximation space $V^A$ depends on parameter $\theta$, where

$$V^A = \left\{ \sum_{\theta} \text{span}(\phi^A_0, \ldots, \phi^A_{N-1}) \right\}$$

yields a richer approximation space.

To solve problem (2), we used a direct eigensolver to find the eigenvector coefficients and eigenvalues $C_n, \tilde{E}_n$, for $n = 0, \ldots, N - 1$. For augmented Hermite bases, the resulting eigenvalues $\tilde{E}_n$ and eigenvectors $C_n$ depend on the parameters $\theta$ of the normalizing flow. Noting that

$$\sum_{n=0}^{N-1} \tilde{E}_n \geq \sum_{n=0}^{N-1} E_n,$$

we used a first-order iterative optimization algorithm to optimize the parameters $\theta$ by minimizing the loss function

$$\mathcal{L} = \sum_{n=0}^{N-1} \tilde{E}_n.$$

For more details on the training procedure, we refer to section 5.

We fixed $d = 1$ and solved (1) with the anharmonic potential $V(x) = \frac{1}{2} x^2 + \frac{1}{4} x^4$. We studied the convergence of both approximation schemes as a function of the truncation parameter, $N$. We considered values of $N$ ranging from 1 to 49. To compute the elements of $\tilde{H}$ we used Gauss-Hermite quadratures see section 5. Figure 1 shows five bands, each of which represents the sum of five eigenvalues in ascending order. The graph clearly shows that both Hermite and augmented Hermite basis functions converge as a function of $N$, with the latter achieving faster convergence. Furthermore, because a Bubnov-Galerkin numerical scheme for a Schrödinger equation based on Hermite functions converges to the true eigenvalues of (1), we conclude that a numerical scheme based on augmented Hermite functions converges to the true solutions. Finally, our proposed numerical scheme enables us to compute many eigenvalues at once. We remark that this cannot be achieved by applying straight forward standard neural networks. We attribute this to the good inductive bias provided by the use of an $L^2$ basis, which constitutes of the quantum harmonic oscillator eigenfunctions.

Figure 2 shows the convergence of the total loss function, i.e., the sum of all eigenvalues for $N = 5, 6, 7, 8, 9$ at each training iteration $t$, plotted for two discretization schemes. We can see that the loss function converges faster for smaller $N$ implying that a larger number of training iterations are required to model a larger number of excited states. The loss function converges rapidly for low-lying states with only few iterations necessary to optimize the nonlinear parameters $\theta$. This demonstrates the high quality of the inductive bias provided by Hermite functions.

Finally, we analyze the convergence rate of both discretization schemes numerically. To this end, we use the concept of Q-convergence, see [9] for details: a sequence $(x_N)_N$ converging to a limit $x^*$ is said to converge Q-super-linearly to $x^*$, iff

$$e_N := \left| \frac{x_N - x^*}{x_{N-1} - x^*} \right| \rightarrow 0 \quad \text{for } N \rightarrow \infty.$$

To define the sequence $(e_N)_N$ for our schemes, we use the second band of eigenvalues (states from 5 to 10) for both discretization schemes, i.e.,

$$x_N = \sum_{n=5}^{10} \tilde{E}_n.$$

The sequence convergence limit is defined as

$$x^* = \sum_{n=5}^{10} E^*_n,$$

where the reference converged eigenvalues $E^*_n$ were computed using a large basis set with $N = 29$. The reference eigenvalues computed with Hermite and augmented Hermite basis sets differ slightly (with $3 \times 10^{-3}$ at maximum) which can be attributed
The average error over bands of five approximate eigenvalues is depicted as a function of the basis truncation parameter $N$. The results are plotted for Hermite (dotted lines) and augmented Hermite (solid lines) discretizations schemes. The color of the lines indicates different energy bands. To improve the contrast between the lines, every other marker is omitted.

The loss as function of the number of training iterations for $N = 5, 6, 7, 8, 9$ (plotted with blue, red, orange, teal, and green). Dotted and solid lines correspond to approximate eigenvalues computed using Hermite and augmented Hermite discretization schemes, respectively. To improve the contrast between the lines, every 5th marker is omitted.

to the properties of the stochastic nonlinear optimizer. Therefore, we choose to define $E_n^*$ based on the converged eigenvalues computed by the respective discretization scheme.

We computed the quantity $e_N$ for different values of $N$. Since the resulting sequence values $\{e_N\}_{N=10}^{N=29}$ are noisy, we fitted a linear regressor to them and plotted the resulting function for the two discretization schemes in Figure 3. Both discretization schemes result in Q-super-linear convergence, with augmented Hermite converging faster. We observed that the convergence of augmented Hermite functions worsens as the accuracy increases, whereas this behavior is absent when discretizing with Hermite functions. We attributed this to the iterative nonlinear optimization performed for augmented Hermite functions, which resulted in the oscillating behavior of the loss function around its extremal points.

For the same size of the linear expansion $N$, the computational costs for performing the numerical simulation above are, indeed, higher when using augmented Hermite functions. This is due to the need for training the normalizing flow and having to compute the trace of the projected Hamiltonian at each step. However, clearly a smaller $N$ is required to converge a certain number of exited states when using augmented Hermite functions than when using Hermite functions.

4 Conclusions and Outlook

Normalizing flows can be used to augment the expressivity of standard basis sets of $L^2$. We show that augmented basis sets define a rich approximation space consisting of a family of parameterized linear spaces that are all dense in $L^2$. We demonstrate the concept’s effectiveness by simulating the eigenfunctions of a perturbed quantum harmonic oscillator using augmented Hermite functions. Our findings indicate quick convergence of the numerical scheme with the size of the basis set. Furthermore, the results were shown to be more accurate than those obtained by using Hermite functions with the same basis size.

Despite the fact that numerical simulations have demonstrated the convergence behavior of augmented basis sets for simulating the eigenfunctions of Hamiltonian operators as $N$ increases, theoretical results are still lacking. Moreover, future work should focus on convergence for a fixed truncation parameter $N$ by increasing the size of the normalizing flow.
This numerical scheme is yet to be used on other high-dimensional differential equations or on more complicated quantum mechanical problems, e.g., simulations of dynamics and spectra of polyatomic molecules, or quantum chemical calculations. In particular, the precision of standard basis sets for approximating solutions of differential equations decreases exponentially as the number of dimensions increase. While augmenting the basis sets with normalising flows reduces the size of the linear expansion $N$ required to achieve a particular level of accuracy, it is unclear whether the curse of dimensionality can be mitigated. Another issue in higher dimensions is the computation of integrals. We used Gauss quadratures in this manuscript, which are not suitable for higher dimensions because their size grows exponentially with the number of dimensions, though sparse grid approaches, such as Smolyak grids, can mitigate the steep scaling for certain problems [10]. Stochastic estimations of integrals, such as Monte-Carlo methods, may provide a dimension-independent scaling at the expense of lower accuracy. Another approach may be the use of collocation methods, which are equivalent to solving the Schrödinger equation by demanding that it is satisfied at a set of points, i.e., no integration is necessary [11]. We believe that augmented basis sets have the potential for accurate modeling of excited states of quantum models with unbounded potentials experiencing a dissociation behavior.

5 Code Availability

The computer code and all relevant data can be obtained from the online repository at https://github.com/CFEL-CMI/FlowBasis.

Supplementary Material

The normalizing flow we used for training has the form

$$g_{\gamma}^{-1}(x) = \tanh(f_{\gamma}(\tanh^{-1}(x - \beta)/\alpha)) + \alpha + \beta,$$

where $f$ is an invertible residual neural network, whose parameters are denoted by $\gamma$. The neural network $f$ is composed of 1 layer with 128 hidden units, with Lipschitz activation functions, i.e., functions of the form

$$\sigma(x) = \frac{1}{1.1} \cdot \frac{x}{1 + \exp(-x)}.$$

Through a fixed scaling procedure, the input to the $\tanh^{-1}$ function is guaranteed to lie within $[-1, 1]$. The free parameters of the normalizing flow $\theta = (\gamma, \alpha, \beta)$ are optimized using the Adam optimization algorithm in [12], with a learning rate $\alpha = 10^{-3}$. To compute the matrix elements of $\hat{H}$ in (2), we used Gauss-Hermite quadratures of order 90. This is possible and convenient since

$$\int \phi_i(g^{-1}(x))V(x)\phi_j(g^{-1}(x))|\det \nabla_x g^{-1}(x)||\ dx = \int \phi_i(x)V(g(x))\phi_j(x)\ dx,$$

e.g., matrix elements of the potential function in the augmented Hermite functions correspond to matrix elements of the perturbed potential $V \circ g$ in the Hermite functions. While the integral on the right hand side contains $V \circ g$, it is still possible to compute accurately with Gauss-Hermite quadratures since the potential in our example is simple and $g$ is a smooth Lipschitz function. Same argumentation can be perused for the kinetic energy operator. Note that the $n$th Hermite functions have $n$ nodes, which means that high-order Hermite functions are harder to integrate. Indeed, we observed that the calculated energies go below the variational limit when using a larger basis set for a fixed order of quadrature points or when using a smaller order.
of quadrature points for the same size of the basis. For the states considered in Figure 1 we observed that using 90 quadrature points was enough for obtaining correct variational limits. Finally, note that the computation of quadrature points using numpy has only been tested up to degree 100. Higher degrees may be problematic, which restricted the size of the basis set that we could consider in this study.

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