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ON DISCRETE LEAST-SQUARES PROJECTION IN UNBOUNDED DOMAIN WITH RANDOM EVALUATIONS AND ITS APPLICATION TO PARAMETRIC UNCERTAINTY QUANTIFICATION*

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Abstract. This work is concerned with approximating multivariate functions in an unbounded domain by using a discrete least-squares projection with random point evaluations. Particular attention is given to functions with random Gaussian or gamma parameters. We first demonstrate that the traditional Hermite (Laguerre) polynomials chaos expansion suffers from the *instability* in the sense that an *unfeasible* number of points, which is relevant to the dimension of the approximation space, is needed to guarantee the stability in the least-squares framework. We then propose to use the Hermite/Laguerre *functions* (rather than polynomials) as bases in the expansion. The corresponding design points are obtained by mapping the uniformly distributed random points in bounded intervals to the unbounded domain, which involved a mapping parameter L. By using the Hermite/Laguerre *functions* and a proper mapping parameter, the stability can be significantly improved even if the number of design points scales *linearly* (up to a logarithmic factor) with the dimension of the approximation space. Apart from the stability, another important issue is the rate of convergence. To speed up the convergence, an effective scaling factor is introduced, and a principle for choosing quasi-optimal scaling factor is discussed. Applications to parametric uncertainty quantification are illustrated by considering a random ODE model together with an elliptic problem with lognormal random input.

Key words. uncertainty quantification, least-squares projection, unbounded domain, Hermite functions, scaling, stability

AMS subject classifications. 41A10, 42C05, 65D05, 65N12

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1. Introduction.

In recent years, there has been a growing need to model uncertainty in mathematical and physical models and to quantify the resulting effect on output quantities of interest (QoI). Several methodologies for accomplishing these tasks fall under the growing subdiscipline of uncertainty quantification (UQ). In general, one can use a probabilistic setting to include these uncertainties in mathematical models. In such a framework, the random input parameters are modeled as random variables; infinite-dimensional analogues leveraging random fields with a prescribed correlation structure extend this procedure to more general settings. Frequently, the goal of this mathematical and computational analysis becomes the prediction of statistical moments of the solution, or statistics of some QoI, given the probability distribution of the input random data.

A fundamental problems in UQ is approximation of a multivariate function $Z = f(x, \mathbf{y})$, where the parameters $\mathbf{y} = (y_1, y_2, \ldots, y_d)$ are d-dimensional random vectors. The function Z might be a solution resulting from a stochastic PDE problem or

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a derived QoI from such a system. Efficient and robust numerical methods that address such problems have been investigated in detail in recent years (see, e.g., [6, 32, 33, 12, 30, 31, 23] and references therein). One of these methods that has enjoyed much attention and success is the generalized polynomial chaos (gPC) method (see, e.g., [32, 33, 12]), which is a generalization of the Wiener–Hermite polynomial chaos expansion [29]. In gPC, we expand the solution Z in polynomials of the input random variables y_i. When Z exhibits regular variation with respect to y_i, gPC yields efficient convergence rates with respect to the polynomial degree of expansion. With intrusive gPC approaches, existing deterministic solvers must be rewritten, and solvers for a coupled system of deterministic equations are needed, which can be very complicated if the underlying differential equations have nontrivial nonlinear form; see, e.g., [32, 6, 36]. By contrast, nonintrusive methods build a polynomial approximation by leveraging only existing deterministic solvers in a Monte-Carlo-like fashion.

To efficiently build a gPC approximation, one can resort to the discrete least-squares projection onto a polynomial space. A major design criterion for this approach is the specification of $\mathbf{y}$ sample locations. There exist a number of popular design grids: randomly generated points, Quasi-Monte Carlo points, specially designed points, etc.; see, e.g., [15, 9, 16, 35]. It is known that obtaining the *optimal* sample design is not straightforward as demonstrated by a recent comparison work in [11]. Analysis for the least-squares approach utilizing random points is addressed in several contexts; see, e.g., [22, 8, 35]. Generally speaking, the least-squares approach is stable when the number of sample points behaves quadratically with the dimension of the approximation space. This quadratic condition can be weakened if we work with the Chebyshev measure [7].

Note that all the above results are for random parameters in *bounded* domains. As far as we have known, there are no exhaustive investigations for problems in unbounded domains, i.e., for functions $f(\mathbf{y})$ with Gaussian or gamma random parameters. In this paper, we will consider the problem of approximating functions with Gaussian or gamma random parameters by using a discrete least-squares projection with random points evaluations. In this case, the traditional approach is to use the so-called Hermite or Laguerre chaos expansions, where the collocation points with respect to the Gaussian or gamma measure will be generated. However, we will show that such an approach suffers from an *instability* in the sense that the corresponding design matrices in the least-squares approach are well conditioned *only* when the number of random points is *exponentially* related to the dimension of the approximation space, i.e., the number of random points equals $(\#\Lambda)^{c\#\Lambda}$ with $\#\Lambda$ being the dimension of the approximation space. This is obviously *unacceptable* for practical computations.

To improve the stability we will propose to use the Hermite (Laguerre) *function* approximation to replace the Hermite (Laguerre) polynomial approach. Then the mapped uniformly distributed random points are used to control the condition number of the design matrix. By choosing a suitable mapping parameter, it is demonstrated numerically that these two strategies will make the condition number small provided that the number of design points is *linearly* proportional to the dimension of the approximation space. This stability result is further justified by a theoretical proof.

The rate of convergence is another serious issue. In fact, approximating a function by Hermite polynomials or functions was rejected by Gottlieb–Orszag ([13, pp. 44–45]). They pointed out that *to study the rate of convergence of Hermite series, we consider the expansion of* $\sin(x)\ldots$. *The result is very bad: to resolve* M *wavelengths of* $\sin(x)$ *requires nearly* M^2 *Hermite polynomials! Because of the poor resolution properties of Hermite polynomials the authors doubt they will be of much practical*

value in applications of spectral methods.

How to improve the resolution property of the Hermite expansion methods? One remedy is to use the so-called scaling factor which expands the underlying function by $h_n(\alpha x)$ instead of $h_n(x)$, where $\alpha > 0$ is a properly chosen constant. In [27], a scaling factor formula combining the size of the solution decay rate and the roots of $h_N(x)$ is proposed, where N is the largest expansion term in the Hermite spectral expansion. Numerical analysis based on asymptotic analysis numerical experiments demonstrate that the use of the scaling factor can indeed provide a significant improvement over the observation of Gottlieb and Orszag. The theoretical justification of the use of the scaling factor proposed in [27] was made in [10, 20]. In particular, Hermite spectral methods are investigated in [20] for linear diffusion equations and nonlinear convection-diffusion equations in unbounded domains. When the solution domain is unbounded, the diffusion operator no longer has a compact resolvent, which makes the Hermite spectral methods *unstable*. To overcome this difficulty, a time-dependent scaling factor is employed in the Hermite expansions, which yields a positive bilinear form. As a consequence, stability is recovered and spectral convergence speed is significantly enhanced. In fact, in the past ten years, the use of the scaling factor proposed in [27] has been used in many areas including computational optics [17], computational astrophysics [24], etc. In particular, the scaling factor formula is included in the recent MATLAB code GSGPEs [4].

When studying uncertainty using the gPC methods, Jardak, Su, and Karniadakis [18] and Xiu and Karniadakis [32] pointed out that the relatively poor resolution properties of Hermite and Laguerre expansions are well documented in [13]. They further pointed out the rescaling procedure as done in [27] can be employed to accelerate convergence. However, the progress of using the scaling factor for the UQ problems has not been great. This is one of the main motivations for the present work. In this work, we will introduce suitable scaling factors to speed up the convergence. Applications to parametric UQ are discussed by considering random ODE models and elliptic-type problems with lognormal random input. A number of numerical examples are provided to confirm the efficiency of the Hermite (Laguerre) function approach with the use of the scaling factors. We summarize here the distinct features of our approach.

- We investigate the discrete least-squares approach for functions with Gaussian or gamma random parameters; applications to UQ are discussed.
- We propose to use the Hermite (Laguerre) functions as the approximation bases, which is different from the traditional Hermite (Laguerre) polynomials. Stability is guaranteed with an acceptable number of evaluation points and relevant theoretical justification is provided.
- We introduce the scaling factor in the least-squares approach to speed up the convergence, and a principle for choosing the scaling is provided. The numerical results indicate that the use of the proposed scaling factor is indeed very useful.

The rest of this paper is organized as follows. In section 2, we introduce the approximation problem of a function in d dimensions by discrete least-squares projection. Some commonly used high-dimensional approximation spaces are discussed. We also show that the Hermite (Laguerre) gPC expansions need an unacceptable number of evaluation points to guarantee the stability. In section 3, we propose to use the Hermite (Laguerre) function approach. Stability under this approach is ensured with the use of mapped uniform random points. Moreover, a useful scaling factor is introduced to speed up the convergence. Applications to parametric UQ are discussed in

section 4. Some conclusions are drawn in the final section.

2. The least-squares projection. In this section, we follow closely the works [22, 8, 35] to give a basic introduction to the discrete least-squares approach, however, please note that we shall focus on problems in unbounded domains.

Let $\mathbf{y} = (y_1, \dots, y_d)^T$ be a vector with d random variables, which takes values in $\Gamma \equiv \mathbb{R}^d$ or $\Gamma \equiv \mathbb{R}_+^d$. We will focus on the cases where $\{y_i\}_{i=1}^d$ are Gaussian random variables ($\Gamma \equiv \mathbb{R}^d$) or gamma random variables ($\Gamma \equiv \mathbb{R}_+^d$). We suppose that the variables $\{y_i\}_{i=1}^d$ are independent with marginal probability density function (PDF) ρ_i for each random variable y_i. The joint PDF is given by $\rho(\mathbf{y}) = \prod_{i=1}^d \rho_i(y_i) : \Gamma \to \mathbb{R}^+$.

Assume that the functions considered in this paper are in the space L_ρ^2 endowed with the norm

$$\|f\|_{L_\rho^2} = \mathbb{E}\left[f^2(\mathbf{y})\right] = \left(\int_\Gamma f^2(\mathbf{y})\rho(\mathbf{y})d\mathbf{y}\right)^{1/2}. \tag{2.1}$$

The purpose is to efficiently build a finite dimension approximation of $f(\mathbf{y})$ or some general functionals $g \circ f$ associated with $f(\mathbf{y})$. To this end, we first choose the one-dimensional orthogonal bases (not only limited to polynomials) with respect to each random variable y^i:

$$\{\phi_j^i\}_{j=1}^\infty \in L_\rho^2, \quad i = 1, \dots, d,$$

where ϕ_j^i is called the jth order basis. Then the multidimensional bases can be formed by tensorizing the univariate bases $\{\phi_j^i\}_{j=1}^\infty$. To explicitly form these bases, let us first define the following multi-index:

$$\mathbf{n} = (n_1, \dots, n_d) \in \mathbb{N}^d \quad \text{with} \quad |\mathbf{n}| = \sum_{i=1}^d n_i.$$

Define the d-dimensional bases $\mathbf{\Phi_n}$ as

$$\mathbf{\Phi_n}(\mathbf{y}) = \prod_{i=1}^d \phi_{n_i}^i(y_i), \tag{2.2}$$

where $\{\phi_{n_i}^i\}_{n_i=1}^\infty$ is the one-dimensional basis. Let $\Lambda \subset \mathbb{N}^d$ be a finite multi-index set, and denote by $N := \#\Lambda$ the cardinality of an index set Λ. The finite-dimensional approximation space defined by Λ is given by

$$\mathbf{P}^\Lambda := \text{span}\{\mathbf{\Phi_n}(\mathbf{y}),\ \mathbf{n} \in \Lambda\}.$$

Throughout the paper, the best approximation of $f(\mathbf{y})$ in $\mathbf{P}^\Lambda$ will be denoted by $P^\Lambda f$, namely,

$$P^\Lambda f := \underset{p \in \mathbf{P}^\Lambda}{\text{argmin}} \|f - p\|_{L_\rho^2}. \tag{2.3}$$

A formula for the best approximation $P^\Lambda f$ involves standard Fourier coefficients with respect to the Φ_n, but these coefficients require high-order moment information for the function f and in general cannot be computed explicitly.

Alternatively, we consider the construction of such an approximation $f^\Lambda \in \mathbf{P}^\Lambda$ for the function $Z = f(\mathbf{y})$ by the least-squares approach. To this end, we compute the

exact function values of f at $\mathbf{y}_1, \ldots, \mathbf{y}_m \in \mathbb{R}^d$ with $m > N$, and then find a discrete least-squares approximation f^Λ by requiring

$$f^\Lambda = P_m^\Lambda f = \operatorname*{argmin}_{p \in \mathbf{P}^\Lambda} \frac{1}{m} \sum_{k=1}^{m} \left(p(\mathbf{y}_k) - f(\mathbf{y}_k)\right)^2. \tag{2.4}$$

We introduce the discrete inner product

$$\langle u, v \rangle_m = \frac{1}{m} \sum_{k=1}^{m} u(\mathbf{y}_k) v(\mathbf{y}_k). \tag{2.5}$$

Remark 2.1. We remark that usually the L^2_ρ-best approximation polynomial is chosen as the approximation basis, which yields the so-called gPC method. For example, the Hermite polynomials are used for functions with Gaussian parameters, and the Laguerre polynomials are suitable for functions with gamma parameters, and so on [33]. In such gPC expansions, a natural way to choose the design points is the random sampling method, that is, the random samples are generated with respect to ρ. Of course, other kinds (nonpolynomial) of orthogonal bases can be used in the least-squares approach.

2.1. Multivariate approximation spaces. Given a basis order q and the dimension parameter $d \in \mathbb{N}$, define the following index sets

$$\Lambda_{\mathbf{P}}^{q,d} := \Big\{ \mathbf{n} = (n_1, \ldots, n_d) \in \mathbb{N}^d : \max_{j=1,\ldots,d} n_j \le q \Big\}, \tag{2.6}$$

$$\Lambda_{\mathbf{D}}^{q,d} := \{ \mathbf{n} = (n_1, \ldots, n_d) \in \mathbb{N}^d : |\mathbf{n}| \le q \}. \tag{2.7}$$

The traditional tensor product (TP) space is defined as

$$\mathbf{P}_q^d := \operatorname{span}\big\{ \mathbf{\Phi}_{\mathbf{n}}(\mathbf{y}) : \mathbf{n} \in \Lambda_{\mathbf{P}}^{q,d} \big\}. \tag{2.8}$$

That is, we require in $\mathbf{P}_q^d$ that the basis order in each variable be less than or equal to q. A simple observation is that the dimension of $\mathbf{P}_q^d$ is

$$\dim(\mathbf{P}_q^d) = \#\Lambda_{\mathbf{P}}^{q,d} = (q+1)^d. \tag{2.9}$$

Note that when $d \gg 1$ the dimension of TP spaces grows very quickly with respect to the degree q, which is the so-called *curse of dimensionality*. As a result, the TP spaces are rarely used in practice when d is large. Alternatively, when d is large, the following total degree (TD) space is often employed instead of using the TP space [23, 31]:

$$\mathbf{D}_q^d := \operatorname{span}\big\{ \mathbf{\Phi}_{\mathbf{n}}(\mathbf{x}) : \mathbf{n} \in \Lambda_{\mathbf{D}}^{q,d} \big\}. \tag{2.10}$$

The dimension of $\mathbf{D}_q^d$ is

$$\dim(\mathbf{D}_q^d) = \#\Lambda_{\mathbf{D}}^{q,d} = \binom{q+d}{d}. \tag{2.11}$$

It is seen that the growth of the dimension of $\mathbf{D}_q^d$ is much slower than that of $\mathbf{P}_q^d$.

Remark 2.2. We remark that the TP and TD spaces are originally defined for polynomial spaces. However, spaces based on general one-dimensional bases can be constructed in the same way. Consequently, we will still use the names TP and TD for the spaces with general bases. Moreover, other types of spaces can also be considered, e.g., the hyperbolic cross spaces [7].

2.2. Algebraic formulation. Consider the approximation in the space $\mathbf{P}^\Lambda = \text{span}\{\mathbf{\Phi_n}\}_{\mathbf{n}\in\Lambda}$ with random samples $\{\mathbf{y}_k\}_{k=1}^m$. If we choose a proper ordering scheme for the multi-index, we can order the multidimensional bases via a single index. For example, we can arrange the index set Λ in lexicographical order, namely, given $\mathbf{n}'$, $\mathbf{n}'' \in \Lambda$

$$\mathbf{n}' < \mathbf{n}'' \Leftrightarrow \big[|\mathbf{n}'| < |\mathbf{n}''|\big] \vee \big[\,(|\mathbf{n}'| = |\mathbf{n}''|) \wedge \big(\exists\, j : n'_j < n''_j \wedge (n'_i = n''_i,\ \forall i < j)\big)\,\big].$$

Then the space $\mathbf{P}^\Lambda$ can be rewritten as $\mathbf{P}^\Lambda = \text{span}\{\{\mathbf{\Phi_n}\}_{j=1}^N\}$ with $N = \#\Lambda$. The least-squares solution can be written

$$f^\Lambda = \sum_{j=1}^N c_j \mathbf{\Phi}_j, \tag{2.12}$$

where $\mathbf{c} = (c_1, \ldots, c_N)^\top$ is the coefficient vector. The algebraic problem to determine the unknown coefficient $\mathbf{c}$ can be formulated as

$$\mathbf{c} = \underset{\mathbf{z}\in\mathbb{R}^N}{\text{argmin}} \|\mathbf{Dz} - \mathbf{b}\|_2, \tag{2.13}$$

where

$$\mathbf{D} = \big(\mathbf{\Phi}_j(\mathbf{y}_k)\big), \quad j = 1, \ldots, N,\ k = 1, \ldots, m,$$

and $\mathbf{b} = [f(\mathbf{y}_1), \ldots, f(\mathbf{y}_m)]^\top$ contains the evaluations of the target function f in the collocation points. The solution to the least-squares problem (2.13) can also be computed by solving an $N \times N$ system, namely,

$$\mathbf{Az} = \mathbf{f} \tag{2.14}$$

with

$$\mathbf{A} := \mathbf{D}^\top\mathbf{D} = \big(\langle \mathbf{\Phi}_i, \mathbf{\Phi}_j\rangle_m\big)_{i,j=1,\ldots,N}, \quad \mathbf{f} := \mathbf{D}^\top\mathbf{b} = \big(\langle f, \mathbf{\Phi}_j\rangle_m\big)_{j=1,\ldots,N}. \tag{2.15}$$

From the computational point of view, we can solve problem (2.13) by using the QR factorization. Alternatively, we can also solve (2.14) by the Cholesky factorization.

2.3. The Hermite (Laguerre) chaos expansion: Stability issue. As was discussed in Remark 2.1, a natural way to approximate functions with Gaussian (gamma) parameters is the Hermite (Laguerre) chaos expansion. In this section, we shall show, by numerical examples, that the least-squares projection with Hermite (Laguerre) polynomial expansion is unstable, in the sense that an unfeasible number of random points, i.e., $m = (\#\Lambda)^{c\#\Lambda}$, are needed to guarantee the stability.

To this end, let us recall that the one-dimensional normalized Hermite polynomials $\{H_k(y)\}_{k=0}^\infty$, defined on the whole line $\mathbb{R} := (-\infty, +\infty)$, are orthogonal with respect to the weight function $\rho^G(y) = \mathrm{e}^{-y^2}$, namely,

$$\int_{-\infty}^{+\infty} \rho^G(y) H_m(y) H_n(y) dy = \delta_{mn}. \tag{2.16}$$

We denote by $\mathbf{H_n}(\mathbf{y})$ the multivariate Hermite polynomial with multi-index $\mathbf{n}$, which was obtained by tensorizing the one-dimensional Hermite polynomials. Then, a natural way to approximate a multivariate function $f^G(\mathbf{y})$ with Gaussian parameters $\mathbf{y}$ is

$$f^G(\mathbf{y}) = \sum_n c_\mathbf{n} \mathbf{H_n}(\mathbf{y}), \quad \mathbf{n} \in \Lambda, \tag{2.17}$$

where Λ is the index set that can be either $\Lambda_\mathbf{P}^{q,d}$ or $\Lambda_\mathbf{D}^{q,d}$.

Similarly, for a function $f^E(\mathbf{y})$ with gamma random parameters $\mathbf{y}$, a natural basis for such an expansion would be the tensorized Laguerre polynomials $\mathbf{L_n}$ that are orthogonal with respect to the weight function $\rho^E(\mathbf{y}) = \prod_{i=1}^d \mathrm{e}^{-y_i}$. More precisely, we expand

$$f^E(\mathbf{Y}) = \sum_n c_{\mathbf{n}} \mathbf{L_n}(\mathbf{y}), \quad \mathbf{n} \in \Lambda. \tag{2.18}$$

Note that we consider here a special type of gamma random parameter y, for which the PDF yields $\rho(y) = \mathrm{e}^{-y}$. Such random variables are also referred to as exponential random variables. More general types of gamma random parameters with PDF

$$\rho^E(y) = \frac{\beta^\alpha y^{\alpha-1} \mathrm{e}^{-\beta y}}{\Gamma(\alpha)} \tag{2.19}$$

can be considered in a similar way, and the corresponding chaos expansion is the generalized Laguerre chaos expansion.

In the least-squares framework, to construct the expansions (2.17) and (2.18), a natural choice of the collocation points $\{\mathbf{y}\}_{i=1}^m$ is to generate random points according to the Gaussian (gamma) measure. In both cases, we can obtain the corresponding design matrices $\mathbf{A}^G$ and $\mathbf{A}^E$, respectively.

We remark that for problems in *bounded* domains, e.g., the uniform random parameters in $[-1, 1]$, the relevant tests have been done by many researchers; see, e.g., [22, 8, 7, 35]. For instance, for the uniform measure in $[-1, 1]$, it is known that a quadratic dependence of the number of random points, i.e., $m = c(\#\Lambda)^2$, is sufficient to guarantee the stability of the least-squares approach. Moreover, if the Chebyshev measure is considered, fewer points are needed to guarantee the stability [7].

What is the difference if the underlying domain is unbounded? The answer is quite negative: the $m = c(\#\Lambda)^2$ quadratic random points cannot guarantee the stability.

We will demonstrate the above claim by testing the condition number of the design matrices, i.e.,

$$\mathrm{cond}(\mathbf{A}) = \frac{\sigma_{max}(\mathbf{A})}{\sigma_{min}(\mathbf{A})}, \quad \mathbf{A} = \mathbf{A}^G \text{ or } \mathbf{A}^E. \tag{2.20}$$

Let us first consider the Hermite chaos expansion (2.17). In this case, the random points are generated with respect to the Gaussian measure. Note that the design matrix is a random matrix. Therefore, in the computations we will repeat the test 100 times, and the *mean* condition number will be reported. In Figure 1, the growth of condition numbers with respect to the polynomial order is shown for the one-dimensional case. It is noted that the condition number admits an exponential growth with respect to the polynomial order, for both the linear dependence $m = c(\#\Lambda)$ (left) and the quadratic dependence $m = c(\#\Lambda)^2$ (right) cases. In fact, similar tests with the dependence $m = c(\#\Lambda)^\nu$ with $3 \le \nu \le 5$ produce results similar to those in Figure 1.

We further consider the Laguerre chaos expansion, which is suitable for approximating functions supported in $\mathbb{R}_+^d$. Note that the corresponding random points are generated by the gamma measure. The bottom of Figure 1 shows the results for one-dimensional tests, which indicate that the condition number of the gamma case grows faster than that in the Gaussian.

Figure 2 presents the two-dimensional tests for both the TP and TD constructions. The left figure is for the Gaussian, while the right one is for the gamma. Again the

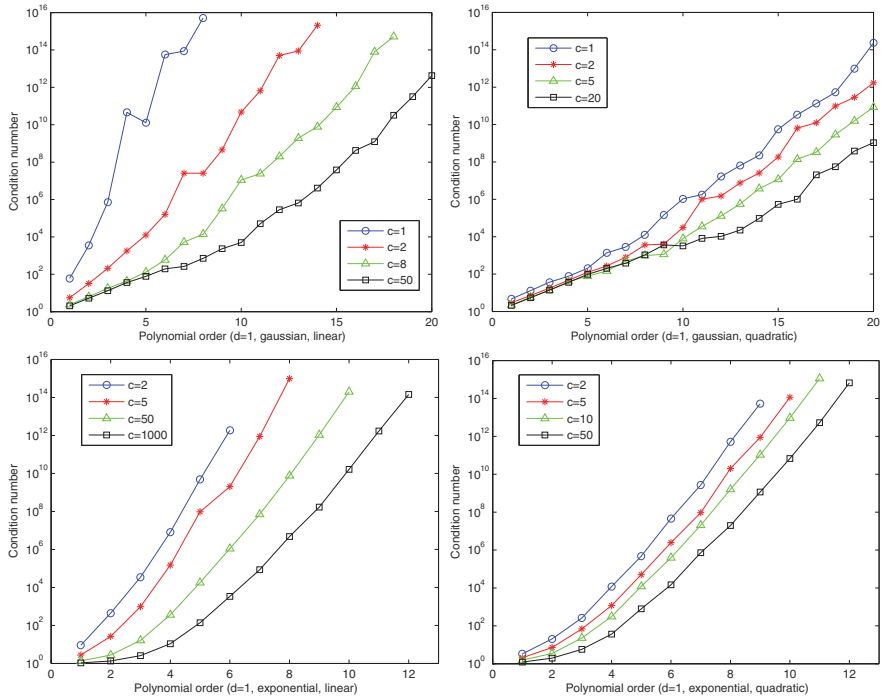

FIG. 1. *Condition numbers with respect to polynomial order in the one-dimensional case, with left for* $m = c(\#\Lambda)$ *and right for* $m = c(\#\Lambda)^2$. *Top: Gaussian case; bottom: gamma case.*

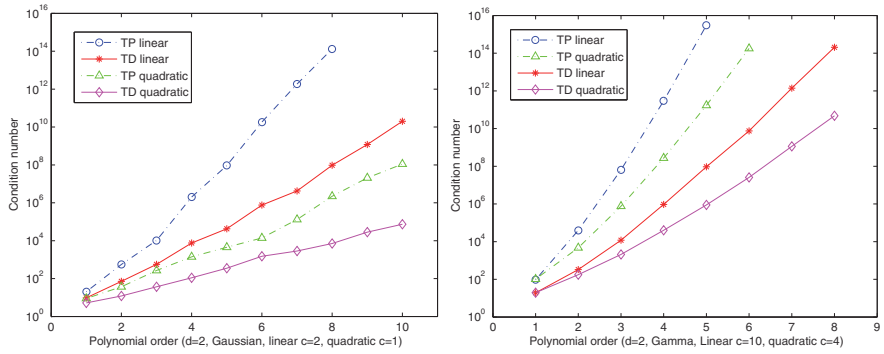

FIG. 2. *Condition numbers with respect to polynomial order in the two-dimensional case. Left: Gaussian; right: gamma.*

exponential growth of the condition number is observed, where it is seen that the TD spaces work better than the TP spaces.

With the above observations, it seems hopeless to control the condition number in the unbounded domain. In fact, to have a good control of the condition number, it is observed in the Ph.D. thesis of Migliorati [21] that an unfeasible number of points with $m = (\#\Lambda)^{c(\#\Lambda)}$ is needed. To improve this, we shall introduce the Hermite (Laguerre) function approach to replace the Hermite (Laguerre) polynomial expansion.

Remark 2.3. We remark that we are not saying that the Hermite (Laguerre) polynomial chaos expansions are unfeasible in the least-squares framework. In fact,

we can still use such approaches with a *small* number of polynomial degrees. In this case, fast convergence can still be expected. However, the convergence rate deteriorates when a large polynomial degree q is used due to the exponential growth of the condition number. Some numerical tests are provided in [21].

3. The Hermite (Laguerre) function expansions. In this section, we propose to use the Hermite (Laguerre) function approximation instead of the traditional Hermite (Laguerre) polynomial approximation. The one-dimensional Hermite functions, also named modified Hermite polynomials, are defined by

$$\tilde{H}_m(y) = \mathrm{e}^{-\frac{y^2}{2}} H_m(y), \quad m = 0, 1, \ldots, \tag{3.1}$$

where $\{H_m(y)\}_{m\geq 0}$ are normalized Hermite polynomials. Note that the Hermite functions are orthogonal in the following sense,

$$\int_{-\infty}^{+\infty} \tilde{H}_m(y)\tilde{H}_n(y)dy = \delta_{mn}. \tag{3.2}$$

The corresponding multivariate Hermite functions $\tilde{\mathbf{H}}_{\mathbf{m}}(\mathbf{y})$ can be defined by tensorizing the one-dimensional Hermite functions.

The Laguerre functions are defined as

$$\tilde{L}_m(y) = \mathrm{e}^{-\frac{y}{2}} L_m(y), \quad m = 0, 1, \ldots, \tag{3.3}$$

where $\{L_m(y)\}_{m\geq 0}$ are Laguerre polynomials. The corresponding multivariate Laguerre functions $\tilde{\mathbf{L}}_{\mathbf{m}}(\mathbf{y})$ can be defined in a similar way. Note that the Hermite/Laguerre functions are no longer polynomials. Nevertheless, in what follows, whenever we use *polynomial order* q it is referring to the qth Hermite/Laguerre function.

It is clear that the Hermite (Laguerre) function expansions are suitable for approximating functions decaying to zero when y goes to infinity. We claim that in UQ applications, we can almost always consider approximating decay functions. To see this, let $f(y)$ (scalar case, for simplicity) be a function with Gaussian parameters that might be the solution of certain stochastic ODEs/PDEs. In the UQ applications, one is interested in some statistical quantities of $f(y)$, such as the kth moment $\int_\Gamma \rho(y) f^k(y)dy$. Let us consider a general expression of such QoI:

$$\mathrm{QoI} = \int_\Gamma \rho(y)(g \circ f)(y)dy, \tag{3.4}$$

where $g \circ f$ is a general smooth functional of $f(y)$. Even if $g \circ f$ is not a decay function, $\rho(y)(g \circ f)$ does, provided that $g \circ f$ grows slower than Gaussian. Thus, we can in fact consider the approximation for $\tilde{f}(y) = \rho(y)(g \circ f)$. As long as a good approximation of $\tilde{f}(y)$ is found, we can get a good approximation for the QoI in (3.4).

Without loss of generality, we can assume that $f(y)$ decays exponentially. Consider the expansion

$$f^G(y) = \sum_{n=0}^{K-1} c_n \tilde{H}_n(y), \quad f^E(y) = \sum_{n=0}^{K-1} c_n \tilde{L}_n(y). \tag{3.5}$$

We are now at the stage to find good collocation points in the least-squares framework. As we have discussed before, the most natural way to find such points is to generate

the samples with respect to the PDF of the random parameters. Moreover, if such a PDF coincides with the weight function of the bases, the expectation of the design matrix would be the identity matrix, and this feature would help in the rigorous stability analysis [8]. In our setting, however, the Hermite (Laguerre) functions are orthogonal with respect to the Lebesgue measure. It is known that it is *impossible* to generate random points with respect to the Lebesgue measure (uniform measure) in unbounded domains. To overcome this difficulty, we shall introduce the mapped uniform samples, which transform the uniform random points $\{\xi_i\}_{i=1}^m$ in $[-1,1]^d$ (or $[0,1]^d$) to $\{y_i\}_{i=1}^m$ in $[-\infty,+\infty]^d$ (or $[0,+\infty]^d$).

Although there exist many feasible mappings, we shall restrict ourselves to a family of mappings defined by

$$y'(\xi) = \frac{L}{(1-\xi^2)^{1+r/2}}, \quad r \geq 0, \tag{3.6}$$

where $L > 0$ is a constant, and r determines how fast the mapping $y(\xi)$ goes to infinity as ξ goes to ± 1; see, e.g., [3, 26] for a thorough discussion on the pros and cons of different mappings. It is easy to verify that

$$y(\xi) = \begin{cases} \frac{L}{2}\log\frac{1+\xi}{1-\xi}, & r=0, \\ \frac{L\xi}{\sqrt{1-\xi^2}}, & r=1, \end{cases} \qquad \xi(y) = \begin{cases} \tanh\left(\frac{y}{L}\right), & r=0, \\ \frac{y/L}{\sqrt{y^2/L^2+1}}, & r=1. \end{cases} \tag{3.7}$$

For other positive integers r, we can always use algebraic computing software to derive the explicit expression of the mapping $y(\xi)$. The mapping with $r = 0$ is often referred to the logarithmic mapping which makes the transformed points decay exponentially, and the mapping with $r > 0$ is referred as algebraic mapping. In our setting, the mapping with $r = 0$ will be used when the Gaussian measure is considered, while the mapping with $r = 1$ will be adopted when the gamma measure is used.

We now summarize our least-squares approach by taking a one-dimensional function with Gaussian parameters as an example. Given the function $f(y)$ to be approximated, i.e., we are interested in the QoI of $\int_{\mathbb{R}} \exp(-y^2/2) f(y) dy$.

- *Step* 1. Motivated by the discussion in the beginning of this section, we seek the following Hermite *function* expansion for $\tilde{f}(y) = \exp(-y^2/2) f(y)$:

$$\tilde{f}(y) = \sum_{k=0}^{K-1} c_i \tilde{H}_k(y). \tag{3.8}$$

- *Step* 2. Let $\mathbf{P}^K := \text{span}\{\tilde{H}^0, \ldots, \tilde{H}^{k-1}\}$. We will find the following least-squares solution

$$f^K = P_m^K f = \underset{p \in \mathbf{P}^K}{\text{argmin}} \sum_{k=1}^m \left(p(y_k) - \tilde{f}(y_k)\right)^2, \tag{3.9}$$

  where the collocation points $\{y_k\}_{k=1}^m$ are chosen as the transformed uniform random points given by the mapping (3.6) with $r = 0$.

This procedure will lead to the desired QoI.

3.1. Stability. In this section, we shall investigate the stability of the least-squares approach by using the Hermite (Laguerre) functions, with mapped uniform

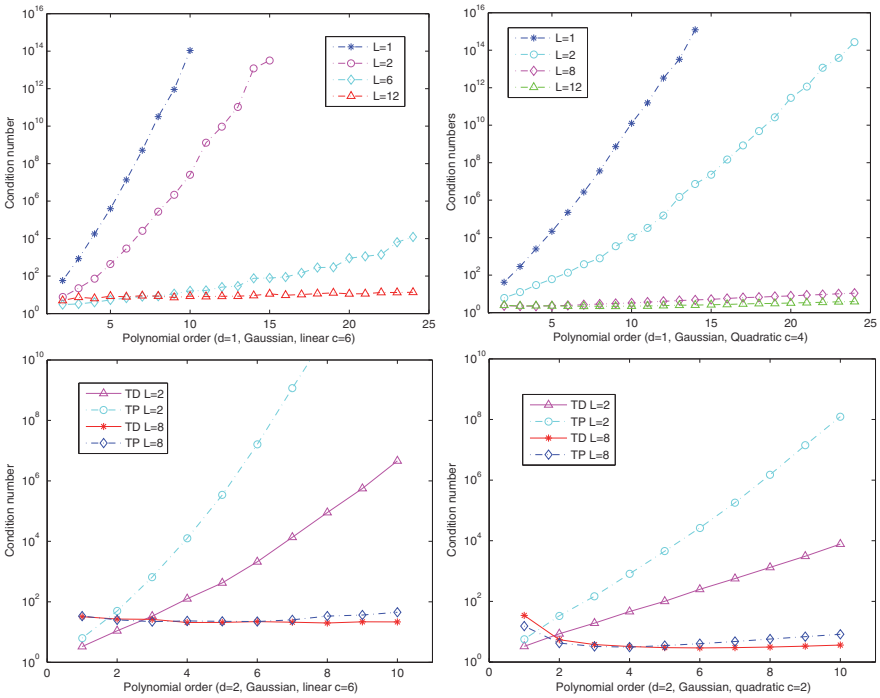

FIG. 3. *Condition numbers with respect to polynomial order. Left is for* $m = 6 * (\#\Lambda)$ *and the right is for* $m = 4 * (\#\Lambda)^2$. *Top: one-dimensional Gaussian; bottom: two-dimensional Gaussian.*

distributed random points. Again, we test the condition number of the corresponding design matrices:

$$\text{cond}(\mathbf{A}) = \frac{\sigma_{max}(\mathbf{A})}{\sigma_{min}(\mathbf{A})}, \quad \mathbf{A} = \mathbf{A}^G \text{ or } \mathbf{A}^E. \tag{3.10}$$

Here we still use $\mathbf{A}$ to avoid too many symbols although we should point out that $\mathbf{A}^G$ ($\mathbf{A}^E$) are evaluations of the Hermite (Laguerre) functions on the mapped random points in $\mathbb{R}^d$ and $\mathbb{R}^d_+$, respectively. As such matrices are random, their condition numbers will be obtained by repeating the test 100 times so that the resulting mean condition number can be obtained. The mean condition number will be used to represent the condition number of the random matrices, which will be reported in the following figures.

In Figure 3, the condition numbers with respect to the bases of order q are given for one-dimensional Hermite function bases. The left plot is devoted to the linear rule with $m = 6 * (\#\Lambda)$, while the right plot is for the quadratic rule with $m = 4 * (\#\Lambda)^2$. In both cases, we can see that using a relatively large transform parameter L, the random matrices $\mathbf{A}$ are well conditioned. The two-dimensional cases are reported in the bottom of Figure 3 for both the TP and the TD spaces. Again, the parameter $L = 8$ results in a well-conditioned design matrix, for both the TP and TD spaces. However, under the same parameter (say $L = 2$), the design matrix of the TD spaces are much better conditioned than that for the TP spaces, which is one of the reasons that the TD space is preferred for higher-dimensional approximation.

Similar numerical tests are carried out for the Laguerre bases and in this case the mapping (3.7) with $r = 1$ is used. The one-dimensional result in the left of Figure 4

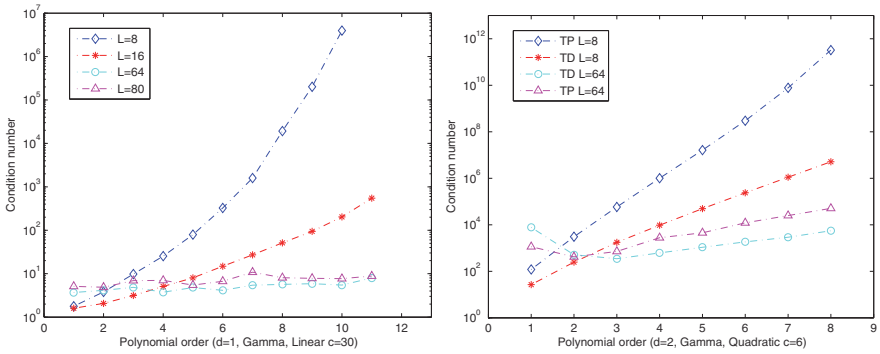

FIG. 4. *Condition numbers with respect to polynomial order. Left: one-dimensional gamma,* $m = 30 * (\#\Lambda)$*; right: two-dimensional gamma,* $m = 6 * (\#\Lambda)^2$.

suggests that the parameter $L = 8$ can no longer guarantee the stability, while a larger parameter (say $L = 64$) will work. The two-dimensional plot is given in the right of the figure. Again, the parameter $L = 64$ results in a better condition number for the design matrices. We also note that more points and larger parameters L are needed for higher-dimensional cases. Moreover, the TD space ($\circ$ and $*$ plots) provide better stability than that of the TP space ($\triangleleft$ and $\diamond$ plots).

We conclude that the design matrix $\mathbf{A}$ can be well conditioned under a set of transformed random points with some relatively large parameter L. As the decay rate for the Gaussian is faster than that for the Laguerre, the transformation parameter L for the Gaussian must be smaller than that for the Laguerre function.

In the following, a rigorous analysis for the stability will be provided. We will only provide the proof for the one-dimensional Hermite functions case; the proof can be extended to the Laguerre case in a straightforward manner.

We first give a lemma concerning the decay properties of the Hermite functions.

LEMMA 3.1. *For any integer* K*, we can find a constant* $\tau(K) > 0$ *such that*

$$|\tilde{H}_k(y)| \le |y|^{-\frac{5}{2}} \quad \forall\, 0 \le k \le K-1, \tag{3.11}$$

provided that $|y| > \tau(K)$.

Proof. Such a simple result is true because for any $t > 0$ we have

$$|\tilde{H}_k(y)| \cdot |y|^t \to 0 \quad \text{when} \quad |y| \to \infty \tag{3.12}$$

due to the involvement of the factor $e^{-\frac{y^2}{2}}$ in the Hermite functions. ∎

We are now ready to prove the stability. Such analysis requires an understanding of how the scaled random matrix $\hat{\mathbf{A}} = L\mathbf{A}$ deviates from its expectation $\mathbb{E}[\hat{\mathbf{A}}]$ in probability $\mathbf{Pr}\{\cdot\}$. Note that the matrix $\hat{\mathbf{A}}$ can be written as

$$\hat{\mathbf{A}} = \mathbf{X}_1 + \mathbf{X}_2 + \cdots + \mathbf{X}_m,$$

where the $\mathbf{X}_i$ are independently and identically distributed copies of the random matrix

$$\mathbf{X} = \frac{L}{m}\big(\tilde{H}_i(y)\tilde{H}_j(y)\big)_{i,j=0,\ldots,K-1}, \tag{3.13}$$

where y is a transformed uniform random variable.

We now state the stability result.

THEOREM 3.2. *The least-squares approach using the Hermite functions* (3.1) *and the transformed uniform random points* (3.7) *is stable in the sense that the scaled design matrix satisfies that* $\forall\, r > 0$

$$\mathbf{Pr}\left\{ |||\hat{\mathbf{A}} - \mathbf{I}||| \geq \frac{5}{8} \right\} \leq 2m^{-r}, \tag{3.14}$$

provided that

$$K \leq \kappa \frac{m}{\log m} \quad \textit{with} \quad \kappa := \frac{c_{1/2}}{(1+r)}, \quad c_{\frac{1}{2}} = \frac{1}{2} + \frac{1}{2}\log\frac{1}{2} > 0, \tag{3.15}$$

and the mapping parameter L *in* (3.7) *satisfies*

$$L > \max\{3\tau(K), 5\sqrt{K}\}, \tag{3.16}$$

where m *is the number of the random points,* K *is the degree of the polynomial.*

Proof. The analysis follows closely with [8] and uses the Chernoff bound [1, 28]. Let $\mathbf{X}_1, \ldots, \mathbf{X}_n$ be independent $K \times K$ random self-adjoint and positive matrices satisfying $\lambda_{max}(\mathbf{X}_i) = |||\mathbf{X}_i||| \leq R$ almost surely, and let

$$\mu_{min} := \lambda_{min}\left(\sum_{i=1}^{m} \mathbb{E}\left[\mathbf{X}_i\right]\right), \quad \mu_{max} := \lambda_{max}\left(\sum_{i=1}^{m} \mathbb{E}\left[\mathbf{X}_i\right]\right).$$

Then, one has for $0 < \delta < 1$

$$\Pr\left\{ \lambda_{min}\left(\sum_{i=1}^{m} \mathbf{X}_i\right) < (1-\delta)\mu_{min} \right\} \leq K\left(\frac{e^{-\delta}}{(1-\delta)^{1-\delta}}\right)^{\mu_{min}/R}, \tag{3.17}$$

$$\Pr\left\{ \lambda_{max}\left(\sum_{i=1}^{m} \mathbf{X}_i\right) > (1+\delta)\mu_{max} \right\} \leq K\left(\frac{e^{\delta}}{(1+\delta)^{1+\delta}}\right)^{\mu_{max}/R}. \tag{3.18}$$

Note that a rank 1 symmetric matrix $ab^T = (b_j a_k)_{j,k=1,\ldots,m}$ has its spectral norm equal to the product of the Euclidean norms of the vectors a and b, and therefore we have

$$|||\mathbf{X}_i||| \leq \frac{1}{m}\sup_{y\in\mathbb{R}} \sum_{i=0}^{K-1} \tilde{H}_i^2 = \frac{M(K)}{m} := R \quad \text{with} \quad M(K) = \sup_{y\in\mathbb{R}} \sum_{i=0}^{K-1} \tilde{H}_i^2(y). \tag{3.19}$$

We are now at the stage to find μ_{min} and μ_{max}. Let

$$\bar{\mathbf{A}} = \mathbb{E}[\hat{\mathbf{A}}] = \sum_{i=1}^{m} \mathbb{E}\left[\mathbf{X}_i\right].$$

Using the definition of the expectation and (3.6), we know that the elements of $\bar{\mathbf{A}}$ satisfy

$$a_{i,j} = \int_{-1}^{1} L\tilde{H}_i\big(y(\xi)\big)\tilde{H}_j\big(y(\xi)\big)d\xi = \int_{\mathbb{R}} \left(1 - \tanh^2\left(\frac{y}{L}\right)\right)\tilde{H}_i(y)\tilde{H}_j(y)dy.$$

Let $V := \operatorname{span}\{\tilde{H}_0, \ldots, \tilde{H}_{K-1}\}$, and

$$a(u,v) = \int_{\mathbb{R}} \left(1 - \tanh^2(y/L)\right) uv dy.$$

The eigenvalues of $\bar{\mathbf{A}}$ are extrema of $a(v,v)$ subject to $\|v\| = 1$, where the norm on v is defined as $\sum c_k^2$. It is easy to verify that $\mu_{max} \le 1$. We now estimate μ_{min}. By letting $v = \sum c_k \tilde{H}_k$ with $\|v\| = 1$, we have

$$a(v,v) \ge \left(1 - \tanh^2(1/3)\right) \int_{-\frac{L}{3}}^{\frac{L}{3}} v^2 dy = \left(1 - \tanh^2(1/3)\right) \left(\int_{\mathbb{R}} v^2 dy - 2\varepsilon \right), \tag{3.20}$$

where

$$\varepsilon = \max\{\varepsilon_+, \varepsilon_-\}, \quad \varepsilon_\pm = \int_{\pm\frac{L}{3}}^{\pm\infty} v^2 dy. \tag{3.21}$$

Straightforward calculations yield

$$\varepsilon_+ = \int_{\frac{L}{3}}^{\infty} v^2 dy \le K^2 \max_i\{c_i^2\} \int_{\frac{L}{3}}^{\infty} y^{-5} dy \le \frac{3^4 K^2}{4L^4}, \tag{3.22}$$

where we have used Lemma 3.1 with $L \ge 3\tau(K)$. If $L > \max\{3\tau(K), 5\sqrt{K}\}$, then by noting that ε_- has the same bound as ε_+ gives

$$\mu_{min} \ge \left(1 - \tanh^2(1/3)\right) \left(1 - \frac{3^4 K^2}{2L^4}\right) \ge \frac{3}{4}. \tag{3.23}$$

Now, we use the Chernoff bound (with $\delta = 1/2$) to obtain

(3.24)

$$\begin{aligned}
\Pr\left\{ \|\|\hat{\mathbf{A}} - \mathbf{I}\|\| > \frac{5}{8} \right\} &\le \Pr\{\lambda_{max}(\hat{\mathbf{A}}) \ge 13/8\} + \Pr\{\lambda_{min}(\hat{\mathbf{A}}) \le 3/8\} \\
&\le \Pr\{\lambda_{max}\hat{\mathbf{A}}) \ge (1+1/2)\cdot 1\} + \Pr\left\{\lambda_{min}(\hat{\mathbf{A}}) \le (1-1/2)\cdot \frac{3}{4}\right\} \\
&\le \Pr\{\lambda_{max}\hat{\mathbf{A}}) \ge (1+1/2)\cdot \mu_{max}\} \\
&\quad + \Pr\{\lambda_{min}(\hat{\mathbf{A}}) \le (1-1/2)\cdot \mu_{min}\} \\
&\le K\left(\frac{\mathrm{e}^{1/2}}{(3/2)^{3/2}}\right)^{\mu_{max}/R} + K\left(\frac{\mathrm{e}^{-1/2}}{(1/2)^{1/2}}\right)^{\mu_{min}/R} \\
&\le 2K\left(\frac{\mathrm{e}^{-1/2}}{(1/2)^{1/2}}\right)^{1/R}.
\end{aligned}$$

Consequently, if we let

$$M(K) \le \kappa \frac{m}{\log m} \tag{3.25}$$

with κ given in (3.15), then the desired result (3.14) can be obtained. By noting that $\tilde{H}_k^2(y) < 1$, we can obtain from (3.19) that $M(K) \le K$. Hence, choosing $M(K) = K$ in (3.25) completes the proof of the theorem. ∎

Note that the requirement (3.16) for L may not be optimal. In fact, inspired by the above proof, we need to choose a large parameter L so that the integral (3.22) is sufficiently small. On the other hand, it is known that the largest root of $\tilde{H}_K$ behaves like $\sqrt{2K}$, so the requirement $L > \sqrt{5K}$ asymptotically coincides with that L should be bigger than the largest root of $\tilde{H}_K$. We also point out that the proof above can be extended to the Laguerre case. However, as the Laguerre functions decay much slower than the Hermite functions, a larger parameter L (approximately the square of the Hermite case) should be used. This can also be estimated by noting that the largest root of $\tilde{L}_K$ behaves like cK.

3.2. Convergence and the scaling factor: Motivation. In this subsection, we shall investigate the convergence issue. By the discussions in the last section, we know that we can use the transformation parameter L to obtain a stable approach. Furthermore, inspired by the proof in [8, 7], one can expect the following convergence property of the least-squares approach:

$$\mathbf{Pr}\Big\{\|f - f_m\|_\rho \geq C \min_{v\in V} \|f - v\|_{L^\infty(\mathbb{R})}\Big\} \leq 2m^{-r}, \tag{3.26}$$

with a suitable norm $\|\cdot\|_\rho$ associated with the transformation $\rho(y) = 1 - \tanh^2(\frac{y}{L})$, where f_m is the least-squares solution. As the proof follows directly the framework of [7], it is thus omitted here. Although the above results imply the error estimate in the finite space V, from the convergence point of view the rate of convergence $(\min_{v\in V} \|f - v\|)$, may depend strongly on properties of the underlying function, such as the regularity and the decay rate.

To this end, we first demonstrate some numerical results for approximating the function $f(y) = 2^{-py^2}$ with a Gaussian parameter y and a constant p. In the following experiments, we will report the error in the L^∞ norm. More precisely, we compute the maximum error on 4000 random grids in $\mathbb{R}$. The approximation error using the Hermite functions against the polynomial order is given in Figure 5. In the computations, the parameter $L = 8$ is used to guarantee the stability. It can be seen from Figure 5 that both the linear rule $m = c(\#\Lambda)$ (right) and the quadratic rule $m = c(\#\Lambda)^2$ (left) produce a very stable approach up to degree $q = 38$.

Another simple observation is that although the function f is sufficiently smooth for any values of p, the convergence rate differs dramatically for p. For $p = 0.6$ ($\circ$ plot), the convergence is very fast, while for $p = 0.2$ or $p = 4$, the convergence is

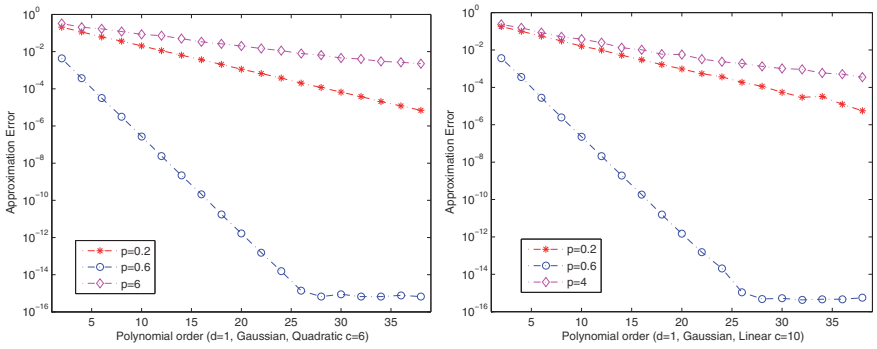

FIG. 5. *Approximation error for $f(y) = 2^{-py^2}$ against the polynomial order with different parameter; p. Left: quadratic rule $m = c * (\#\Lambda)^2$ with $c = 6$; right: linear rule with $c = 10$.*

very slow (yet still stable). This is due to the use of the Hermite functions which behave approximately like $e^{-y^2/2}$ at infinity. It is noted that when the approximated function $f(y)$ matches such a decay property (e.g., $p = 0.6$ which is close to 0.5), the convergence is fast, while the convergence is very slow when the approximated function decays much faster or much slower than the Gaussian function (e.g., $p = 0.2$ or 4). A remedy to fix the above problem is the use of the so-called scaling factor [25, 27]. In spectral methods, the scaling factor is often used to speed up the convergence for approximating functions that decay fast at infinity. Such an idea was successfully applied to the studies of different problems [20, 19, 4].

We now introduce the basic idea of the scaling factor. To this end, let $f(y)$ be a function that decay exponentially, namely,

$$|f(y)| < \epsilon \quad \forall\, |y| > M, \tag{3.27}$$

where $0 < \epsilon \ll 1$ and $M > 0$ are some constants. The idea of using the scaling factor is to expand f as

$$f(y) = \sum_{n=0}^{K-1} c_n \tilde{H}_n(\alpha y) \Leftrightarrow f\left(\frac{y}{\alpha}\right) = \sum_{n=0}^{K-1} c_n \tilde{H}_n(y), \tag{3.28}$$

where $\alpha > 0$ is a scaling factor. The key issue of using α is to scale the points $\{y_i\}$ so that y_i/α are well within the effective support of f.

To see the effect of the scaling, let us carry out some numerical tests. We first consider a fast decay function $f(y) = 2^{-6y^2}$. In the top of Figure 6, the maximum approximation error with respect to polynomial order is shown for the one-dimensional case. In the left of the figure, we fix the parameter $L = 8$ to ensure stability. It is noticed that the convergence for the original Hermite function approach ($\alpha = 1$, $\circ$ plot) is very slow (although stable), while the use of a scaling factor α indeed can significantly improve the convergence rate. In this example, the optimal scaling factor seems to be around $\alpha = 2.8$ ($*$ plot). The right of the figure presents the convergence properties using the scaling $\alpha = 2.8$ but with variate parameters L. It is noticed that, under small parameters ($L = 0.5$ or 1), the convergence rate deteriorates when a large polynomial order is used. This is due to the instability when small parameters L are used. In contrast, the parameter $L = 8$ ($\diamond$ plot) results in a very stable approach.

Let us now consider a slowly decaying function $\tilde{f}(y) = 2^{-0.2y^2}$. The corresponding convergence results are shown in the bottom of Figure 6. The bottom left uses the fixed parameter $L = 8$ and several values of α. It is noticed that the optimal scaling factor in this case is about $\alpha = 0.82$ ($*$ plot) in terms of rate of convergence, although the results for all α are stable. The bottom right shows the error curves using the optimal scaling $\alpha = 0.82$ but with various parameters L. It is noticed that with small parameters ($L = 1$ or 2, $*$ and $\circ$ plots) the convergence rate deteriorates when large polynomial order is used. In contrast, the parameter $L = 8$ ($\diamond$ plot) results in a very stable approach.

3.3. Scaling factor: Application to least-squares approach. The above tests suggest that proper scaling factors should be employed to speed up the rate of convergence. We now discuss how to find a feasible scaling in our least-squares approach. Note that the numerical solution (the expansion coefficients $\mathbf{c}$) satisfies

$$\mathbf{Ac} = \mathbf{f} \tag{3.29}$$

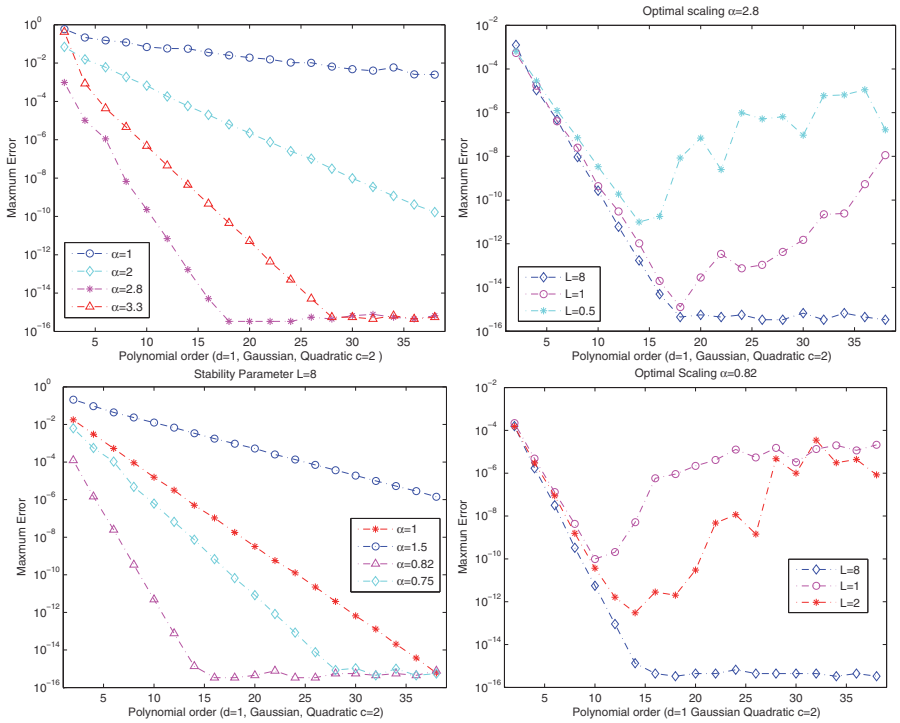

FIG. 6. *Convergence with respect to polynomial order (one-dimensional Gaussian with* $m = 2*(\#\Lambda)^2$*). Top:* $f(y) = 2^{-6y^2}$*. Left uses different scaling* α *with transformation parameter* $L = 8$*, and right uses the optimal scaling* $\alpha = 2.8$ *with different parameter* L*. Bottom:* $f(y) = 2^{-0.2y^2}$*. Left uses different scaling* α *with transformation parameter* $L = 8$*, and right uses the optimal scaling* $\alpha = 0.82$ *with different parameter* L*.*

with $\mathbf{A}$ being the design matrix, where

$$\mathbf{A} = \left(\langle \tilde{H}_i, \tilde{H}_j \rangle_m\right)_{i,j=1}^N, \quad \mathbf{f} = \left(\langle f, \tilde{H}_j \rangle_m\right)_{j=1}^N. \tag{3.30}$$

For ease of discussion, we assume that the points $\{y_i\}_{i=1}^m$ are in absolute increase order, i.e.,

$$|y_1| \le |y_2| \le \cdots \le |y_m|.$$

Note that

$$\mathbf{f}_k = \langle f, H_k \rangle_m = \sum_{i=1}^m f\left(\frac{y_i}{\alpha}\right) H_k(y_i), \quad k = 1, \ldots, N. \tag{3.31}$$

Clearly, in order to compute $\{c_k\}_{k=1}^N$, we need to use information of f from the interval $[-M, M]$ out of which the contribution of f is 0 in the sense of the floating number. This observation suggests that

$$\max_{1\le j\le m} \{|y_j|\}/\alpha \le M \quad \Rightarrow \quad \alpha = \max_{1\le j\le m} \{|y_j|\}/M. \tag{3.32}$$

This idea is similar to the proposal given in [27] in the context of pseudospectral methods. However, in our least-squares approach the points $\{y_i\}_{i=1}^m$ are generated

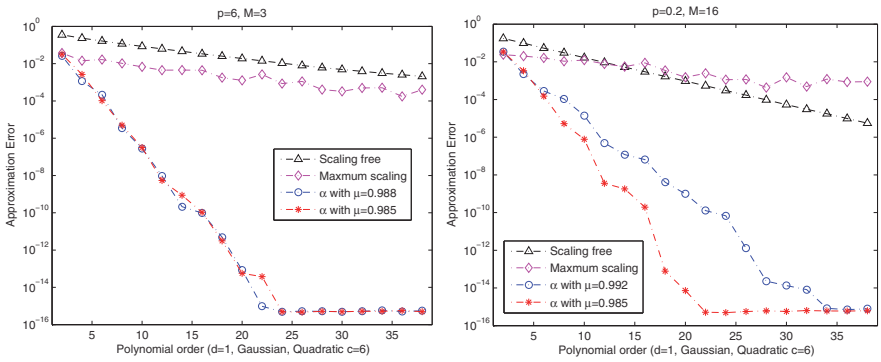

FIG. 7. *Error against polynomial order* ($f(y) = 2^{-py^2}$, *one-dimensional Gaussian,* $m = 6 * (\#\Lambda)^2$). *Left:* $p = 6$ *with different scaling* α*; right:* $p = 0.2$ *with different scaling* α.

randomly. The scaling α in (3.32) may not be efficient from the probability point of view: there is the possibility that only a few points (maybe only 2 or 3) are extremely large (we refer to such points as *bad points*), which means that the scaling (3.32) may *overscale* the points. This motivates us to *drop* such *bad points*. More precisely, we choose

$$\tilde{\alpha} = \max_{1 \le j \le \tilde{m}} \{|y_j|\}/M, \quad \tilde{m} = \lfloor \mu m \rfloor, \tag{3.33}$$

where μ is a parameter close to 1. That is, we drop $m - \lceil \mu m \rceil$ possible *bad points*, and require $\lfloor \mu m \rfloor$ points to contribute to the computation of $\{c_k\}_{k=1}^N$. In practice, it is found that we can just set $\mu \sim 98\%$, meaning that the probability of generating bad points is 2%.

We now repeat the numerical test in Figure 6 (the left ones), with particular attention to the use of the scalings (3.32) and (3.33). The numerical results are given in Figure 7, where *scaling free* stands for the results without using a scaling, *maximum scaling* denotes the scaling computed by (3.32), while *scaling with* $\mu = s\%$ means that the scaling is computed by (3.33). The left of Figure 7 shows the convergence for approximating $\tilde{f}(y) = 2^{-6y^2}$. In this case, we simply set $M = 3$, i.e., the effective support of $f(y)$ is chosen as $[-3, 3]$. It can be seen that the numerical error with scaling factor (3.33) decays very quickly ($*$ and $\circ$ plots) as compared to the *scaling-free* case ($\triangleright$ plot), while the results with *maximum scaling* ($\diamond$ plot) behave almost the same as the *scaling-free* case. The right plot is for $\tilde{f}(y) = 2^{-0.2y^2}$, and we set $M = 16$ for this test. A similar phenomenon is observed.

For high-dimensional cases, a reasonable scaling should be chosen in each direction. A two-dimensional test is provided in Figure 8. The function to be approximated is $\tilde{f}(y) = \mathrm{e}^{-4(y_1^2+y_2^2)}\sin(y_1 + y_2)$, and the approximating space is the TD space. In the left plot, we have used the linear rule $m = 10 * (\#\Lambda)$, while the quadratic rule with $m = 2 * (\#\Lambda)^2$ is used in the right plot. The scaling factors are computed by (3.33) with $M = 2.5$. It is shown that the convergence is stable, and the scaling works very well. Furthermore, it is noticed that the convergence rate of the quadratic rule (right) is better than the linear rule. This might be due to that the linear rule uses fewer points than the quadratic rule.

Remark 3.3. In practice, finding the optimal parameter M is not straightforward due to the limit information of the function f. Nevertheless, we can always find a reasonable M if the information for f is reasonably sufficient. It remains a research

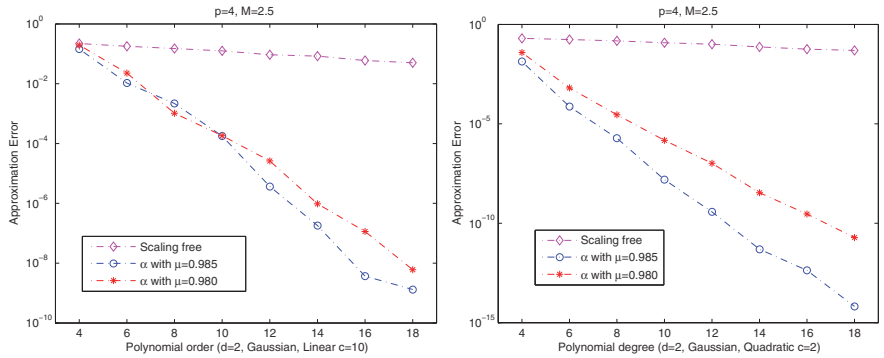

FIG. 8. *Numerical error against polynomial order* ($\tilde{f}(y) = e^{-4(y_1^2+y_2^2)} sin(y_1 + y_2)$, $M = 2.5$, *TD space.) Left: the linear rule with* $m = 10 * (\#\Lambda)$ *Right: the quadratic rule with* $m = 2 * (\#\Lambda)^2$.

issue on how to find an acceptable M if only a few evaluations of f are available; we will leave this problem for future studies.

4. Parametric UQ: Illustrative examples. In this section, we discuss the application of the least-squares Hermite (Laguerre) approximations to parametric uncertainty analysis; precisely, we shall use the least-squares approach based on the Hermite (Laguerre) functions to compute the QoI of UQ problems.

4.1. A simple random ODE. We first consider a simple random ODE problem with gamma random input:

$$\frac{df}{dt} = -k(y)f, \quad f(0) = 1, \tag{4.1}$$

where $k(y)$ is a function with respect to a random gamma parameter y. Note that for such problems with gamma random input, the Laguerre functions will be used as the bases. To illustrate the idea, we set $k(y) = \beta y$. We are interested in the second moment of the solution, i.e.,

$$\text{QoI} = \int_{\mathbb{R}_+} \mathrm{e}^{-y} f^2(t, y) dy.$$

Note that in the least-squares approach, for each random point y_i, one has to solve the ODE to get the information $f(t, y_i)$. The random points that are located in $(0, \infty)$ and used here are the transformed uniform random points. We will use the mapping (3.6) with parameters $r = 1$ and $L = 64$ to guarantee the stability. The numerical convergence results are shown ($t = 1$) in Figure 9. The left plots are for $\beta = 1.5$. Note that we are in fact approximating the function $\tilde{f} = \mathrm{e}^{-y} f^2(t, y) = \mathrm{e}^{-4yt}$. It is noticed from Figure 9 that the convergence is very slow without using a scaling, and this is again due to the fast decay of f compared to the gamma measure. In this test, both the *maximum scaling* and the *scaling with* $\mu = s\%$ work well, which is different from the observations for the Gaussian measure. It is likely due to the slow decay of the gamma measure, which results in a very large effective support (outside of the effective support $\tilde{f}$ is 0 with machine accuracy), and thus, the probability of *overscale* is not so large as in the Gaussian case. The right plot is for $\beta = -0.65$. Again, all scaling values work well, although the scaling computed by (3.33) behaves more stable.

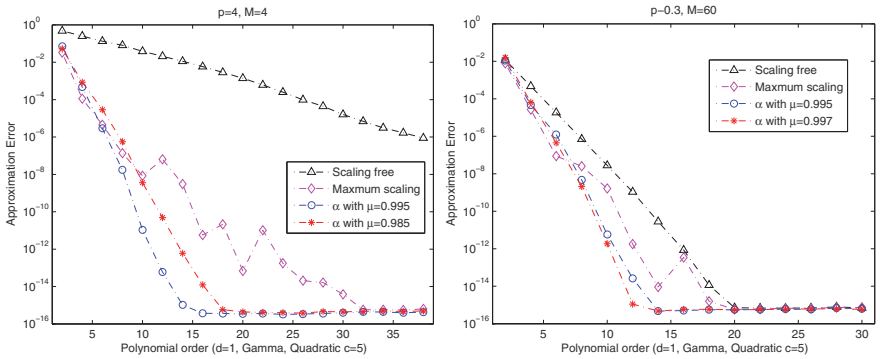

FIG. 9. *Problem* (4.1)*: convergence with respect to polynomial order with* $m = 5 * (\#\Lambda)^2$*. Left:* $\beta = 2$*, with different scaling* α*; right:* $\beta = -0.65$*, with different scaling* α*.*

It is seen from the above example that for problems with gamma random parameters the *maximum scaling* can be used. Moreover, if the partial maximum scaling associated with parameter μ is used, then larger μ (say $\mu = 0.995$) should be used. This is quite different from the Gaussian case.

4.2. Elliptic problems with lognormal random input. We now take the following elliptic problems with lognormal random input as an example:

$$-\nabla \cdot (a(x,\omega)\nabla u) = f, \quad x \in D, \ \ \omega \in \Omega, \tag{4.2}$$
$$u(x,\omega)|_{\partial D} = 0.$$

The coefficient $a(x,\omega) : \vec{D} \times \Omega \to \mathbb{R}$ is a lognormal random field, i.e.,

$$a(x,\omega) = \mathrm{e}^{\gamma(x,\omega)}, \quad \gamma(x,\omega) \sim N(\mu,\sigma^2) \quad \forall x \in D, \tag{4.3}$$

where $N(\eta,\sigma^2)$ denotes a Gaussian probability distribution with expected value η and variance σ^2, and $\gamma(x,\omega) : D \times \Omega \to \mathbb{R}$ is such that for $x, x' \in D$ the covariance function $C_\gamma(x,x') = \mathbb{C}\mathrm{ov}[\gamma(x,\cdot)\gamma(x',\cdot)]$ depends only on the distance $\|x - x'\|$ (isotropic property). The lognormal problem (4.2) has been widely investigated in [2, 5, 14].

Here, we consider the least-squares approach to obtain the QoI of problem (4.2) with a finite parameter random coefficient:

$$a^N(x,\omega) \approx \bar{a}(x) + \sum_{i=1}^{N} \sqrt{\lambda_i} y_i(\omega) a_i(x). \tag{4.4}$$

Let us first have a close observation at the following simple case:

$$-\nabla \cdot (e^{cy}\nabla u) = \sin(\pi x), \tag{4.5}$$

where y is a Gaussian random variable and p is a constant. The exact solution is $u = e^{-cy}\sin(\pi x)/\pi^2$. In our least-squares framework, we wish to expand the function

$$\tilde{u} = e^{-\frac{y^2}{2}} u = e^{-\frac{(y+c)^2}{2}} e^{\frac{c^2}{2}} \frac{\sin(\pi x)}{\pi^2},$$

which admits similar decay property to the density function $e^{-y^2/2}$. Consequently, a scaling is *not* needed and the standard Hermite *function* approximation without

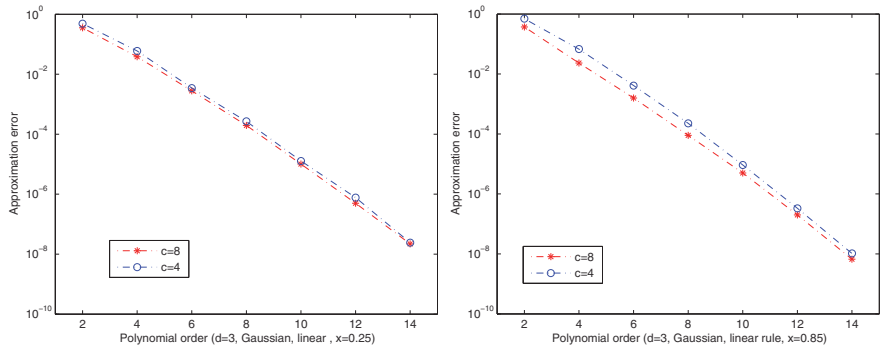

FIG. 10. *Problem* (4.2) *with random coefficient* (4.6)*: convergence with respect to polynomial order with the linear rule* $m = c * (\#\Lambda)$. *Left:* $x_0 = 0.25$*; right:* $x_0 = 0.85$.

scaling should work. In fact, it follows from the maximum principle that the solutions of (4.5) or (4.4)) are bounded. Therefore, a Hermite function approach without scaling should work well.

We now consider problem (4.2) with the following random coefficient

$$a^N(x,\omega) = y_0 + \frac{1}{2}\big(y_1\cos(\pi x) + y_2\sin(\pi x)\big), \quad x \in [0,1], \tag{4.6}$$

with $y_i \sim N(0,1), i = 0,1,2$. That is, three Gaussian parameters are used. We believe that the exact solution of this problem has a Gaussian decay profile similar to the above simple illustration, and we will use the least-squares approximation with the nonscaling Hermite function approach. Suppose we are interested in the QoI

$$\text{QoI} = \int_\Gamma e^{-\frac{\mathbf{y}^2}{2}} u^2(x_0,\mathbf{y})d\mathbf{y}. \tag{4.7}$$

In the computations, the elliptic equations are solved by a standard finite element method. As the exact solution is not available, we use a high level sparse grid collocation method to obtain the reference solution. The numerical error using the least-squares approximation with respect to the bases order is shown in Figure 10. The linear rule $m = c * (\#\Lambda)$ is used, and different x_0 are considered. As discussed above, the Hermite function approach without scaling indeed works well; even the linear rule gives a very good convergence rate.

We close this section by pointing out that only two illustrative examples are provided to demonstrate the performance of the least-squares approximation with Hermite (Laguerre) functions for solving the UQ problems. In fact, practical problems in UQ can be very complicated, and we may need to solve problems with very high dimensional parameters. An alternative way to handle high dimensional problems is to use the ℓ^1-minimization framework [34] instead of the least-squares approach. However, such a framework relies on the assumption that the solution admits a certain *sparse* structure, and this will be part of our future studies.

5. Conclusions. In this paper, we investigate the problem of approximating multivariate functions in unbounded domains by using discrete least-squares projection with random points evaluations. We first demonstrate that the traditional Hermite (Laguerre) polynomials chaos expansion suffers from the numerical instability in

the sense that an *unpractical* number of points, i.e., $(\#\Lambda)^{c\#\Lambda}$, is needed to guarantee the stability in the least-squares framework. To improve this, we propose to use the Hermite (Laguerre) *functions* approach. Then the mapped uniformly distributed random points are used to control the condition number of the design matrices. It is demonstrated that with the Hermite (Laguerre) functions approach the stability can be much improved, even if the number of design points scales *linearly* with the dimension of the approximation space. On the other hand, for problems involving exponential decay the convergence may be very slow due to the poor convergence property of the Hermite (Laguerre) polynomial/function approach. To improve this, scaling factors are investigated to accelerate the convergence rate. This is particularly useful if the underlying function to be approximated decay much faster or much slower than that of the Gaussian (Gamma) measure. A principle for choosing the quasi-optimal scaling factor is provided. Applications to parametric UQ problems are illustrated.

We emphasize that for approximating multivariate functions in unbounded domains by using discrete least-squares projection two parameters are involved: one is the transformation parameter L in (3.6), and another is the scaling factor α in (3.28). The transformation parameter L is used to control the stability while the scaling factor α is used to control the rate of convergence. In this work, as the sample points in the least square approach are generated randomly, an idea of dropping bad points is used, which lead to a useful formula (3.33). There are, however, a number of important issues deserving further attention, which are listed below.

- *Optimal scaling.* The scaling factor α given in section 3.2 is determined by the size of the effective support, i.e., M. If the data information is sufficiently large then M can be easily obtained. In the UQ problems large data information means a significant amount of computational time for solving differential equations. One possible remedy is to use less accurate but fast (even parallel) solvers, as a rough M should serve the purpose. This remains to be examined.
- *High dimensions.* If the underlying solution admits certain *sparsity* structure, we may use the ℓ^1-minimization framework instead of the least-squares approach to further enhance the computational efficiency. This topic with suitable transformation and scaling should be studied.

We finally remark that the use of Hermite functions in the approximation is somehow equivalent to introducing a pre-conditioner in the algebraic formulation (2.13), and we will discuss this topic further in our future work.

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