

# DFG-Schwerpunktprogramm 1324

„Extraktion quantifizierbarer Information aus komplexen Systemen“

## Stochastic Galerkin Matrices

O. G. Ernst, E. Ullmann

Preprint 32



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# STOCHASTIC GALERKIN MATRICES\*

OLIVER G. ERNST<sup>†</sup> AND ELISABETH ULLMANN<sup>†</sup>

**Abstract.** We investigate the structural, spectral and sparsity properties of Stochastic Galerkin matrices as arise in the discretization of linear differential equations with random coefficient functions. These matrices are characterized as the Galerkin representation of polynomial multiplication operators. In particular, it is shown that the global Galerkin matrix associated with complete polynomials cannot be diagonalized in the stochastically linear case.

**Key words.** Stochastic Galerkin method, stochastic finite elements, orthogonal polynomials.

**AMS subject classifications.** 65N30, 65C30, 15A18

**1. Introduction.** As a technique for propagating data uncertainty through the numerical solution of partial differential equations (PDEs), stochastic finite element methods have received considerable attention in recent years. The introduction of a Galerkin discretization scheme based on polynomials in random variables by Ghanem and Spanos [13] led both to a wide adoption of this method among practitioners as well as systematic investigation of the mathematical properties of these schemes. The basic approach of such *Stochastic Galerkin (SG) methods* is a variational formulation in which trial and test spaces consist of random fields rather than deterministic functions, which are formally described as tensor products of functions of deterministic variables (usually space and/or time) on one hand, and functions of a number of random variables on the other. For linear partial differential equations with a stochastic differential operator, the resulting Galerkin matrices are sums of tensor products of matrices, of which one factor is associated with the deterministic, the other with the stochastic function space. For nearly all SG discretizations, the stochastic factors, to which we refer as *Stochastic Galerkin matrices*, are of the same highly structured form, and certain practical questions naturally arise when devising efficient solution algorithms for the Galerkin equations, in particular as the global matrix is typically very large, its dimension being the product of the number of degrees of freedom in the deterministic and stochastic function spaces, respectively.

In this paper we address three issues. The first concerns the choice of basis functions in the stochastic space leading to a desirable form of the resulting matrices. It is known that, when using *tensor product polynomials*, a basis can be constructed for which the resulting combined deterministic-stochastic Galerkin matrix is block diagonal (cf. [5, 6]). We show that this is not the case when the more popular subspace of *complete polynomials* are used. Moreover, for the diagonalizable case, we show how this basis can be constructed by solving a small tridiagonal eigenvalue problem. Another issue, arising in the design of iterative solution methods for SG equations, is the determination of the eigenvalues of the Stochastic Galerkin matrices. Here we give a partial result covering the stochastically linear case and an additional order in the stochastically nonlinear case in addition to spectral inclusion bounds and symmetry properties. Finally, we investigate the sparsity structure of the Stochastic Galerkin matrices.

The paper is organized as follows: in Section 2 we describe the Stochastic Galerkin discretization based on both spaces of multivariate tensor product and complete polynomials in random variables and derive the associated Stochastic Galerkin matrices, displaying their basic Kronecker product structure and how their entries may be computed using recurrence relations for orthogonal polynomials. Section 3 shows that a well-known diagonalization procedure used in conjunction with tensor product polynomials does not extend to the smaller space of complete polynomials. Eigenvalues

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and eigenvalue bounds are given in Section 4 and Section 5 gives results on the sparsity structure of Stochastic Galerkin matrices.

**2. Stochastic Galerkin matrices.** In this section we describe the two most commonly occurring types of Stochastic Galerkin matrices, whose entries consist of the expectation of the product of two or three multivariate polynomials in random variables, respectively.

The point of departure is the representation of random fields (see [2] or [7] for an introduction), which constitute the input data for SG discretizations, as finite separated expansions

$$a(x, \boldsymbol{\xi}) = \bar{a}(x) + \sum_{\substack{\boldsymbol{\alpha} \in \mathcal{I}_a, \\ |\boldsymbol{\alpha}| > 0}} a_{\boldsymbol{\alpha}}(x) \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}). \quad (2.1)$$

The deterministic variable  $x$ , which usually represents spatial coordinates and/or time, lies in a bounded domain  $D \subset \mathbb{R}^d$  of dimension  $d$ , and the function  $\bar{a} : D \rightarrow \mathbb{R}$  denotes the expectation of the random field  $a$ . The second variable  $\boldsymbol{\xi} = \boldsymbol{\xi}(\omega)$  is a vector of a finite number  $M \in \mathbb{N}$  of independent centered random variables  $\xi_m : \Omega \rightarrow \mathbb{R}$ ,  $m = 1, \dots, M$ , with unit variance associated with a probability space  $(\Omega, \mathcal{A}, P)$ , consisting of the abstract set  $\Omega$  of elementary events, a  $\sigma$ -algebra  $\mathcal{A}$  on  $\Omega$  and a probability measure  $P$  on  $\mathcal{A}$ . We make the general assumption that all random variables that occur have finite second moments and denote the Hilbert space of such random variables by  $L_P^2(\Omega)$ . Finally,  $\boldsymbol{\alpha} \in \mathbb{N}_0^M$  denotes a multi-index varying in an index set  $\mathcal{I}_a$  with  $|\boldsymbol{\alpha}| := \alpha_1 + \dots + \alpha_M$ , and  $\psi_{\boldsymbol{\alpha}}$  denotes a polynomial in the variables  $\xi_1, \dots, \xi_M$ . Denoting the range of the  $m$ -th random variable  $\xi_m$  by  $\Gamma_m := \xi_m(\Omega)$  and  $\Gamma := \Gamma_1 \times \dots \times \Gamma_M$ , we have  $\boldsymbol{\xi}(\omega) \in \Gamma$  for all  $\omega \in \Omega$ .

In the following we shall suppress the deterministic variable  $x$  and view  $a = a(\boldsymbol{\xi})$  simply as a random variable taking values in a finite-dimensional space of functions. This is sufficient for our purpose of studying the properties of the matrices obtained after Galerkin discretization. Moreover, we mention a special case of the expansion (2.1) which occurs frequently in applications and in which only *linear* polynomials in  $\boldsymbol{\xi}$  appear in the expansion, which then takes on the form

$$a(\boldsymbol{\xi}) = \bar{a} + \sum_{m=1}^M a_m \xi_m. \quad (2.2)$$

We refer to this situation as the (*stochastically*) *linear case*.

The space of polynomials  $\psi_{\boldsymbol{\alpha}}$  is determined by fixing the multi-index set  $\mathcal{I}_a$ . We distinguish the cases of *tensor product polynomials*

$$\mathcal{I}_a = \mathcal{I}_p := \{\boldsymbol{\alpha} \in \mathbb{N}_0^M : \alpha_j \leq p, \text{ for all } j = 1, \dots, M\}$$

of individual degree at most  $p$  and that of *complete polynomials*

$$\mathcal{I}_a = \mathcal{I}_p^C := \{\boldsymbol{\alpha} \in \mathbb{N}_0^M : |\boldsymbol{\alpha}| \leq p\} \subseteq \mathcal{I}_p$$

of total degree at most  $p$ . Introducing the multivariate polynomial spaces

$$\mathcal{V}_p := \text{span}\{\boldsymbol{\xi}^{\boldsymbol{\alpha}} : \boldsymbol{\alpha} \in \mathcal{I}_p\} \quad \text{and} \quad \mathcal{V}_p^C := \text{span}\{\boldsymbol{\xi}^{\boldsymbol{\alpha}} : \boldsymbol{\alpha} \in \mathcal{I}_p^C\},$$

where  $\boldsymbol{\xi}^{\boldsymbol{\alpha}}$  denotes the  $M$ -variate monomial  $\xi_1^{\alpha_1} \xi_2^{\alpha_2} \dots \xi_M^{\alpha_M}$ , it is easily verified that  $\mathcal{V}_p^C \subseteq \mathcal{V}_p$  and

$$N_p := \dim \mathcal{V}_p = (1+p)^M \quad \text{and} \quad N_p^C := \dim \mathcal{V}_p^C = \binom{M+p}{p}. \quad (2.3)$$

**2.1. Galerkin equations.** The matrices under study arise from a Galerkin discretization of the equation  $au = f$  with given random functions  $a$  and  $f$ , resulting in the discrete variational problem of finding  $u \in \mathcal{V}$  such that

$$\langle a(\boldsymbol{\xi})u(\boldsymbol{\xi})v(\boldsymbol{\xi}) \rangle = \langle f(\boldsymbol{\xi})v(\boldsymbol{\xi}) \rangle \quad \forall v \in \mathcal{V}, \quad (2.4)$$

where  $\mathcal{V}$  is either  $\mathcal{V}_p$  or  $\mathcal{V}_p^C$  and  $\langle \xi \rangle$  denotes the expectation of the random variable  $\xi$ . We note that (2.4) is the abstract representation of a SG formulation in which the functions of the random vector  $\boldsymbol{\xi}$  can be interpreted to take values either in a function space appropriate for the underlying continuous variational setting or, after discretization in the deterministic variable, a finite-dimensional vector space. Assuming further that each of the independent random variables  $\xi_m$  has a probability density  $\rho_m : \Gamma_m \rightarrow \mathbb{R}_0^+$ , their joint density  $\rho : \Gamma \rightarrow \mathbb{R}_0^+$  is given by the product  $\rho = \prod_{m=1}^M \rho_m$  and we may write

$$\langle u(\boldsymbol{\xi}) \rangle = \int_{\Gamma} u(\boldsymbol{\xi}) \rho(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int_{\Gamma_1} \dots \int_{\Gamma_M} u(\xi_1, \dots, \xi_M) \rho_M(\xi_M) d\xi_M \dots \rho_1(\xi_1) d\xi_1.$$

Moreover, instead of  $L_p^2(\Omega)$ , we may equivalently consider the weighted  $L^2$ -space  $L_\rho^2(\Gamma)$ . Inserting a representation  $u = \sum_{\beta} u_{\beta} \psi_{\beta}$  of  $u$  with respect to a basis  $\Psi := \{\psi_{\beta}\}$  of  $\mathcal{V}$  in (2.4) and requiring the variational equation to hold for each test function  $\psi_{\gamma}$ ,  $\gamma \in \mathcal{I}$ , we arrive at the linear system of equations

$$\mathbf{G}u = f$$

associated with (2.4) and the basis  $\Psi$ , where the Galerkin matrix  $\mathbf{G} \in \mathbb{R}^{N \times N}$ , with  $N = N_p$  for  $\mathcal{V} = \mathcal{V}_p$  or  $N = N_p^C$  for  $\mathcal{V} = \mathcal{V}_p^C$ , respectively, has the form

$$\mathbf{G} = \bar{a}\mathbf{G}_0 + \sum_{|\alpha| > 0} a_{\alpha} \mathbf{G}_{\alpha} \quad (2.5)$$

with matrices whose entries associated with each multi-index pair  $(\beta, \gamma) \in \mathcal{I} \times \mathcal{I}$  are given by

$$[\mathbf{G}_0]_{\beta, \gamma} = \langle \psi_{\beta} \psi_{\gamma} \rangle \quad \text{and} \quad [\mathbf{G}_{\alpha}]_{\beta, \gamma} = \langle \psi_{\alpha} \psi_{\beta} \psi_{\gamma} \rangle, \quad \alpha \in \mathcal{I}_a, |\alpha| > 0. \quad (2.6)$$

Note that we distinguish the index sets  $\mathcal{I}_a$  for the coefficient field from that for the basis functions  $\mathcal{I}$ ; we shall see later that there are reasons for choosing the former larger than the latter. In the stochastically linear case only the  $M$  multi-indices with  $|\alpha| = 1$  occur in the sum and, indexing these with  $m = 1, 2, \dots, M$ , the Galerkin matrices in this case are simply

$$[\mathbf{G}_m]_{\beta, \gamma} = \langle \xi_m \psi_{\beta} \psi_{\gamma} \rangle, \quad \beta, \gamma \in \mathcal{I}, \quad m = 1, 2, \dots, M. \quad (2.7)$$

We note that the structure of the matrices  $\mathbf{G}_{\alpha}$  as given in (2.6) reveals that these represent multiplication operators on the multivariate polynomial spaces  $\mathcal{V}_p$  and  $\mathcal{V}_p^C$ , respectively. More precisely, denoting by  $P_{\mathcal{V}} : L_\rho^2(\Gamma) \rightarrow \mathcal{V}$  the orthogonal projection onto either  $\mathcal{V} = \mathcal{V}_p$  or  $\mathcal{V} = \mathcal{V}_p^C$ , respectively, as well as by  $M_{\alpha}$  the linear operator which maps a polynomial  $\psi \in \mathcal{V}$  to the product  $\psi_{\alpha} \psi$  with a fixed basis element  $\psi_{\alpha}$ ,  $\alpha \in \mathcal{I}_a$ , then the stochastic Galerkin matrix  $\mathbf{G}_{\alpha}$  represents the operator

$$P_{\mathcal{V}} M_{\alpha} : \mathcal{V} \rightarrow \mathcal{V}, \\ \psi \mapsto P_{\mathcal{V}}(\psi_{\alpha} \psi)$$

with respect to the basis  $\Psi$ .

**2.2. Choice of basis.** The construction of a basis of multivariate polynomials is most easily accomplished using suitable univariate polynomials. A convenient approach is based on the univariate orthonormal polynomials  $\{\psi_j^{(m)}(\xi_m)\}_{j \in \mathbb{N}_0}$  associated with each of the probability densities  $\rho_m$  as weight functions, such that

$$\langle \psi_i^{(m)} \psi_j^{(m)} \rangle = \left( \psi_i^{(m)}, \psi_j^{(m)} \right)_{L^2_{\rho_m}(\Gamma_m)} := \int_{\Gamma_m} \psi_i^{(m)}(\xi) \psi_j^{(m)}(\xi) \rho_m(\xi) d\xi = \delta_{i,j}, \quad i, j \in \mathbb{N}_0.$$

PROPOSITION 1. *Given  $p \in \mathbb{N}_0$ , the (possibly unbounded) intervals  $\Gamma_m = [a_m, b_m]$  as well as probability densities  $\rho_m$  supported on  $\Gamma_m$ , then the set of multivariate polynomials*

$$\Psi := \{\psi_\alpha : \alpha \in \mathcal{I}\}, \quad \psi_\alpha(\boldsymbol{\xi}) := \prod_{m=1}^M \psi_{\alpha_m}^{(m)}(\xi_m), \quad (2.8)$$

where  $\{\psi_j^{(m)}\}_{j=0}^p$  denote the first  $p+1$  orthonormal polynomials with respect to the probability density  $\rho_m$ , form an orthonormal basis of  $\mathcal{V}_p$  for  $\mathcal{I} = \mathcal{I}_p$  as well as of  $\mathcal{V}_p^C$  for  $\mathcal{I} = \mathcal{I}_p^C$ .

*Proof.* In view of

$$\langle \psi_\alpha \psi_\beta \rangle = \prod_{m=1}^M \left( \psi_{\alpha_m}^{(m)}, \psi_{\beta_m}^{(m)} \right)_{L^2_{\rho_m}(\Gamma_m)} = \prod_{m=1}^M \delta_{\alpha_m, \beta_m}$$

orthonormality follows directly from that of the univariate polynomials. That the polynomials (2.8) form a basis is seen by comparing dimensions.  $\square$

Note that the fact that the  $\rho_m$  are probability densities implies that  $(1, 1)_{L^2_{\rho_m}(\Gamma_m)} = 1$  for all  $m$ , hence the orthonormal polynomial of degree zero is always  $\psi_0^{(m)}(\xi_m) \equiv 1$ . Moreover, the assumption that each random variable has zero mean and unit variance implies

$$(1, \xi_m)_{L^2_{\rho_m}(\Gamma_m)} = \langle \xi_m \rangle = 0, \quad (\xi_m, \xi_m)_{L^2_{\rho_m}(\Gamma_m)} = \langle \xi_m^2 \rangle = 1, \quad (2.9)$$

and therefore we must have  $\psi_1^{(m)}(\xi_m) = \xi_m$  for all  $m$ .

The construction of the bases for  $\mathcal{V}_p$  and  $\mathcal{V}_p^C$  in Proposition 1 is based on the representation of random fields in terms of *independent* random variables  $\xi_1, \dots, \xi_M$ . A more general approach, which is beyond the scope of this paper, can be found in [23], where the expansion of random fields is carried out in terms of statistically dependent random variables. A further alternative approach which employs wavelet bases in place of polynomials in random variables has been proposed by Le Maître et al. [16, 17].

**2.3. Kronecker structure.** To fix the matrix representation of the  $\mathbf{G}_\alpha$  we now introduce an enumeration of the basis polynomials, i.e., of the index sets  $\mathcal{I}_p$  and  $\mathcal{I}_p^C$ . We number the multi-indices  $(\alpha_1, \dots, \alpha_M) \in \mathcal{I}_p$  associated with the tensor product polynomials lexicographically, with  $\alpha_1$  varying the most rapidly. We derive the ordering of the multi-indices  $(\alpha_1, \dots, \alpha_M) \in \mathcal{I}_p^C$  associated with the complete polynomials from that of the tensor product polynomials by simply deleting in the former ordering all multi-indices in  $\mathcal{I}_p \setminus \mathcal{I}_p^C$ . An example is given in Table 2.1.

The Kronecker product structure of the Stochastic Galerkin matrices (2.6) follows directly from the definition (2.8) of the multivariate orthonormal basis polynomials and is summarized below. Given the probability densities  $\{\rho_m\}_{m=1}^M$ , the associated sequences  $\{\psi_n^{(m)}\}$  of orthonormal polynomials and  $p \in \mathbb{N}_0$ , we denote by  $U_n^{(m)}$  the  $(p+1) \times (p+1)$  matrices

$$[U_n^{(m)}]_{i,j} := \left\langle \psi_n^{(m)} \psi_i^{(m)} \psi_j^{(m)} \right\rangle, \quad 1 \leq m \leq M, \quad 0 \leq i, j \leq p, \quad n \in \mathbb{N}_0, \quad (2.10)$$



TABLE 2.1

Enumeration of  $\mathcal{V}_p^C$  as derived from lexicographic ordering of  $\mathcal{V}_p$  for the case  $M = 2$ ,  $p = 3$ . Note that the polynomials in  $\mathcal{V}_p \setminus \mathcal{V}_p^C$  occur in contiguous blocks as  $\alpha_1$  varies.

$\alpha = (\alpha_1, \alpha_2)$	$\psi_\alpha$	$\in \mathcal{V}_3^C ?$
(0,0)	$\psi_0(\xi_1)\psi_0(\xi_2)$	✓
(1,0)	$\psi_1(\xi_1)\psi_0(\xi_2)$	✓
(2,0)	$\psi_2(\xi_1)\psi_0(\xi_2)$	✓
(3,0)	$\psi_3(\xi_1)\psi_0(\xi_2)$	✓
(0,1)	$\psi_0(\xi_1)\psi_1(\xi_2)$	✓
(1,1)	$\psi_1(\xi_1)\psi_1(\xi_2)$	✓
(2,1)	$\psi_2(\xi_1)\psi_1(\xi_2)$	✓
(3,1)	$\psi_3(\xi_1)\psi_1(\xi_2)$	×
(0,2)	$\psi_0(\xi_1)\psi_2(\xi_2)$	✓
(1,2)	$\psi_1(\xi_1)\psi_2(\xi_2)$	✓
(2,2)	$\psi_2(\xi_1)\psi_2(\xi_2)$	×
(3,2)	$\psi_3(\xi_1)\psi_2(\xi_2)$	×
(0,3)	$\psi_0(\xi_1)\psi_3(\xi_2)$	✓
(1,3)	$\psi_1(\xi_1)\psi_3(\xi_2)$	×
(2,3)	$\psi_2(\xi_1)\psi_3(\xi_2)$	×
(3,3)	$\psi_3(\xi_1)\psi_3(\xi_2)$	×

associated with each set of univariate polynomials.

PROPOSITION 2. *The Stochastic Galerkin matrices  $\mathbf{G}_\alpha$  in (2.6) for  $|\alpha| > 0$  obtained for the basis (2.8) of the tensor product polynomial space  $\mathcal{V} = \mathcal{V}_p$  are given by*

$$\mathbf{G}_\alpha = U_{\alpha_M}^{(M)} \otimes \cdots \otimes U_{\alpha_2}^{(2)} \otimes U_{\alpha_1}^{(1)}. \quad (2.11)$$

For  $|\alpha| = 0$  we have  $\mathbf{G}_\alpha = \mathbf{I}_N$ . Moreover for  $|\alpha| = 1$  with  $\alpha_m = 1$  we obtain

$$\mathbf{G}_\alpha = \mathbf{G}_m = I_{p+1} \otimes \cdots \otimes I_{p+1} \otimes U_1^{(m)} \otimes I_{p+1} \otimes \cdots \otimes I_{p+1}, \quad (2.12)$$

in which the univariate matrix  $U_1^{(m)}$  from (2.10) is the  $m$ -th factor (from the right) of the Kronecker product.

*Proof.* Relation (2.11) follows from (2.6) due to the independence of the random variables  $\{\xi_m\}_{m=1}^M$ , as a result of which all integrals decouple to products of one-dimensional integrals. The order of the Kronecker product in (2.11) results from the lexicographic ordering we have fixed for the multi-index set  $\mathcal{S}_p$ , in which  $\alpha_1$  varies most rapidly. Relation (2.12) follows from the orthonormality of the univariate polynomials  $\psi_j^{(m)}$ , as a result of which  $U_0^{(m)} = I_{p+1}$ .  $\square$

When passing from tensor product polynomials to the space of complete polynomials  $\mathcal{V} = \mathcal{V}_p^C$  the matrices  $\mathbf{G}_\alpha$  lose their Kronecker product structure since  $\mathcal{V}_p^C$ —in contrast to  $\mathcal{V}_p$ —is not a tensor product space. One can, however, describe the matrix structure in terms of the tensor product case by making use of the fact that, since the multivariate polynomial basis (2.8) of  $\mathcal{V}_p^C$  is a subset of the corresponding basis of  $\mathcal{V}_p$ , the stochastic Galerkin matrix  $\mathbf{G}_\alpha$  associated with  $\mathcal{V}_p^C$  is a principal submatrix of that obtained for  $\mathcal{V}_p$ .

The following characterization of the structure of the Stochastic Galerkin matrices obtained for complete polynomials in the stochastically linear case generalizes a result given in [21, Lemma 3.1].

LEMMA 3. *For the stochastically linear case, denote the Stochastic Galerkin matrices obtained for the multivariate polynomial basis (2.8) of the space of complete polynomials  $\mathcal{V}_p^C$  by  $\mathbf{G}_m^C$ ,  $m = 0, 1, \dots, M$ . Then*

- (a)  $\mathbf{G}_0^C = \mathbf{I}_N$ .  
(b) For  $m = 1, \dots, M$  each matrix  $\mathbf{G}_m^C$  is permutation-similar to a block-diagonal matrix consisting of  $\binom{M-1+p}{p}$  diagonal blocks each of which is a leading principal submatrix of the univariate matrix  $U_1^{(m)}$  given in (2.10). The first block, and only this, contains the entire matrix  $U_1^{(m)}$ .

*Proof.* Assertion (a) follows by orthonormality of the basis polynomials  $\psi_\beta$ .

We next consider the case  $m = 1$  and show that  $\mathbf{G}_1^C$  is block diagonal with blocks as described in assertion (b). Indeed,  $\mathbf{G}_1^C$  is a principal submatrix of the corresponding matrix  $\mathbf{G}_1$  from the tensor product polynomial basis, which is block diagonal (cf. (2.12)), with a diagonal block  $U_1^{(1)} \in \mathbb{R}^{(p+1) \times (p+1)}$  repeated  $(p+1)^{M-1}$  times along the diagonal:

$$\mathbf{G}_1 = I_{p+1} \otimes \cdots \otimes I_{p+1} \otimes U_1^{(1)} = I_{(p+1)^{M-1}} \otimes U_1^{(1)}. \quad (2.13)$$

We obtain  $\mathbf{G}_1^C$  from  $\mathbf{G}_1$  by deleting the rows and columns associated with multi-indices in  $\mathcal{I}_p \setminus \mathcal{I}_p^C$ , i.e., to basis polynomials with total degree exceeding  $p$ . Note that each diagonal block  $U_1^{(1)}$  of (2.13) corresponds to a range of multi-indices  $(\alpha_1, \tilde{\alpha}) \in \mathcal{I}_p$  with a fixed subindex  $\tilde{\alpha} \in \mathbb{N}_0^{M-1}$  and  $\alpha_1$  ranging from 0 to  $p$ . We distinguish two cases: if  $|\tilde{\alpha}| > p$ , then all multi-indices of this block lie outside  $\mathcal{I}_p^C$  and therefore all associated rows and columns of  $\mathbf{G}_1$  are deleted. If, on the other hand,  $|\tilde{\alpha}| \leq p$ , then the multi-indices  $(\alpha_1, \tilde{\alpha})$  with  $0 \leq \alpha_1 \leq p - |\tilde{\alpha}|$  are retained. According to the ordering we have introduced for the basis polynomials of  $\mathcal{Y}_p$  and  $\mathcal{Y}_p^C$  (cf. Table 2.1), this is a contiguous set of rows and columns from the beginning of a diagonal block, thus leaving a leading principal submatrix of  $U_1^{(1)}$  in the corresponding diagonal block of  $\mathbf{G}_1^C$ . In summary, in passing from  $\mathbf{G}_1$  to  $\mathbf{G}_1^C$ , some diagonal blocks are deleted and those remaining are replaced by leading principal submatrices with order ranging from 0 to  $p$ . Order  $p$  is obtained only for  $|\tilde{\alpha}| = 0$ , i.e., the first block. The number of remaining blocks is given by the number of multi-indices  $\tilde{\alpha}$  of length  $M-1$  such that  $|\tilde{\alpha}| \leq p$ , which is  $\binom{M-1+p}{p}$ .

The remaining cases  $|\alpha| = 1$ ,  $\alpha_m = 1$  with  $m > 1$  follow by the same argument after permuting  $\mathbf{G}_m$  and  $\mathbf{G}_m^C$  in such a way that the multi-indices  $\alpha_1$  and  $\alpha_m$  are interchanged. This corresponds to a reordering of the basis polynomials resulting from the exchange of the independent variables  $\xi_1$  and  $\xi_m$ .  $\square$

**2.4. Matrix entries.** Since the Stochastic Galerkin matrices  $\mathbf{G}_\alpha$  are built up from the univariate matrices  $U_n^{(m)}$ , consisting of Kronecker products (2.11) of these in case of the tensor product polynomial space  $\mathcal{Y}_p$  and principal submatrices of these in case of the complete polynomial space  $\mathcal{Y}_p^C$ , analysis of their entries leads us to investigate the matrices  $U_n^{(m)}$ , i.e., the triple products

$$\left\langle \psi_n^{(m)} \psi_i^{(m)} \psi_j^{(m)} \right\rangle, \quad 0 \leq i, j \leq p, \quad m = 1, \dots, M, \quad n \in \mathbb{N}_0. \quad (2.14)$$

The product  $\psi_i^{(m)} \psi_j^{(m)}$  of two orthonormal polynomials from which the basis (2.8) is constructed, is a polynomial of exact degree  $i+j$ . Therefore there exist coefficients  $g_{kij}^{(m)}$  such that

$$\psi_i^{(m)} \psi_j^{(m)} = \sum_{k=0}^{i+j} g_{kij}^{(m)} \psi_k^{(m)}. \quad (2.15)$$

By orthonormality we must have  $g_{kij}^{(m)} = \left\langle \psi_k^{(m)} \psi_i^{(m)} \psi_j^{(m)} \right\rangle$ . In particular,  $g_{kij}^{(m)} = 0$  whenever  $k > i+j$ .

**PROPOSITION 4.** *The univariate Galerkin matrices  $U_n^{(m)}$  with respect to the orthonormal polynomials with degree  $\leq p$  associated with the weight function  $\rho_m$  are identically zero for  $n > 2p$ .*

As a consequence of Proposition 4, the appropriate multi-index set  $\mathcal{I}_a$  from which the expansion of the input random field  $a$  is constructed in (2.1) is given by  $\mathcal{I}_a = \mathcal{I}_{2p}$  for the tensor product case ( $\mathcal{I} = \mathcal{I}_p$ ) and  $\mathcal{I}_a = \mathcal{I}_{2p}^C$  for complete polynomials ( $\mathcal{I} = \mathcal{I}_p^C$ ). For this choice one obtains the *full* Galerkin projection in (2.4) even when the expansion of the input random field consists of an infinite number of terms. This fact was, to the authors' knowledge, first observed by Matthies and Keese in [19].

The task of computing the coefficients  $g_{kij}^{(m)}$  in (2.15) is known in the orthogonal polynomials literature as the *linearization of products problem*, see [4, Lecture 5]. The linearization coefficients for the orthonormal polynomials associated with common probability density functions can be found in the appendix, where several explicit formulas for these coefficients are collected. We note that this problem has quite a long history, see e.g. [1, 9].

We single out the special case of the univariate matrices (2.10) obtained for  $n = 1$ , namely

$$[U_1^{(m)}]_{i,j} = \left\langle \xi \psi_i^{(m)}(\xi) \psi_j^{(m)}(\xi) \right\rangle = \int_{\Gamma_m} \xi \psi_i^{(m)}(\xi) \psi_j^{(m)}(\xi) \rho_m(\xi) d\xi, \quad 0 \leq i, j, \leq p.$$

From the well-known three-term recurrence satisfied by real orthonormal polynomials

$$\sqrt{\beta_{j+1}} \psi_{j+1}(\xi) = (\xi - \alpha_j) \psi_j(\xi) - \sqrt{\beta_j} \psi_{j-1}(\xi), \quad j = 0, 1, \dots, \quad \psi_{-1} \equiv 0, \quad (2.16)$$

(see e.g. [11, Definition 1.30 and Theorem 1.27]), where we have omitted the superscript  $(m)$ , we observe that

$$U_1^{(m)} = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \\ \sqrt{\beta_1} & \alpha_1 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & \sqrt{\beta_p} & \\ & & & \sqrt{\beta_p} & \alpha_p \end{bmatrix} \quad (2.17)$$

is the Jacobi matrix of recurrence coefficients of the orthonormal polynomials associated with the weight function  $\rho_m$ . It is, in particular, well known that the coefficients  $\sqrt{\beta_j}$  are positive numbers and that the eigenvalues of  $U_1^{(m)}$  are the distinct real zeros of the orthonormal polynomial of degree  $p+1$  associated with weight function  $\rho_m$ . Moreover, these zeros are contained in the support of  $\rho_m$ .

**3. Diagonalization in the stochastically linear case.** When stochastic Galerkin discretizations are applied to PDEs with random data, see e.g. [13, 24, 5, 19], the  $N$  stochastic degrees of freedom are coupled in a tensor product fashion to, say,  $N_x$  deterministic degrees of freedom, resulting in global stochastic-deterministic Galerkin matrices of potentially very large dimension  $N_x \cdot N$ . Since the solution process entails solving linear systems of equations with this coefficient matrix, decoupling these equations will result in substantial computational savings. For the stochastically linear case (2.7) with tensor product polynomials a change of basis under which the Stochastic Galerkin matrices become diagonal was introduced in [5, Section 7]. In coupled stochastic-deterministic formulations this results in block diagonal coefficient matrices, each block being of the size of one deterministic problem, which is reminiscent of Monte-Carlo simulation.

In this section we recall the diagonalizing change of basis, give a simplification for the eigenvalue calculations involved in its construction, and show that diagonalization is not possible for complete polynomial spaces. Throughout this section we consider only the stochastically linear case and employ the notation  $\mathbf{G}_m$ ,  $m = 0, 1, \dots, M$  introduced in (2.7).

To diagonalize the matrices  $\mathbf{G}_m$  we pass from the orthonormal basis  $\Psi$  given in (2.8) to a new basis  $\widehat{\Psi}$  of  $\mathcal{V}_p$  or  $\mathcal{V}_p^C$ , respectively, and denote the resulting Stochastic Galerkin matrices by  $\widehat{\mathbf{G}}_m$ ,  $m = 0, \dots, M$ . In order that  $\widehat{\mathbf{G}}_0$ , which is just the Gramian matrix of  $\widehat{\Psi}$  with respect to

the  $L^2_\rho(\Gamma)$ -inner product, be diagonal, we see that  $\widehat{\Psi}$  must again consist of orthogonal multivariate polynomials, and we again take them to be normalized. Denoting by  $\Psi = [\psi_1, \psi_2, \dots, \psi_N]$  and  $\widehat{\Psi} = [\widehat{\psi}_1, \widehat{\psi}_2, \dots, \widehat{\psi}_N]$  the basis functions arranged as row vectors, the change of basis between the orthonormal bases  $\Psi$  and  $\widehat{\Psi}$  is effected by an orthogonal matrix  $V \in \mathbb{R}^{N \times N}$  such that  $\widehat{\Psi} = \Psi V$ . As a result, the Stochastic Galerkin matrices of the two bases are related by

$$\widehat{G}_m = V^\top G_m V, \quad m = 0, 1, \dots, M. \quad (3.1)$$

We thus arrive at the problem of finding an orthogonal matrix  $V$  which simultaneously diagonalizes the matrices  $\{G_m\}_{m=0}^M$ , a task known as *simultaneous diagonalization by orthogonal congruence*, see [14, Section 4.5]. Since (3.1) represents a spectral decomposition, this problem is equivalent to finding a common system of orthogonal eigenvectors of the matrices  $G_m$ .

**3.1. Tensor product polynomials.** For the tensor product polynomial space  $\mathcal{Y}_p$  with basis (2.8) it is apparent from the structure of the matrices  $G_m$  as given in (2.12) that the matrix

$$V = V_M \otimes V_{M-1} \otimes \dots \otimes V_1 \quad (3.2)$$

simultaneously diagonalizes all matrices  $G_m$  if, and only if, the  $m$  orthogonal matrices  $\{V_m\}_{m=1}^M$  satisfy

$$U_1^{(m)} V_m = V_m \Lambda_m, \quad m = 1, \dots, M, \quad (3.3)$$

with diagonal matrices  $\{\Lambda_m\}_{m=1}^M$ , i.e., if the columns of  $V_m$  are the orthonormal eigenvectors of  $U_1^{(m)}$ . From their definition in (2.10) the matrices  $U_1^{(m)}$  are given by

$$[U_1^{(m)}]_{i,j} = \langle \xi_m \psi_i^{(m)} \psi_j^{(m)} \rangle, \quad i, j = 0, 1, \dots, p, \quad m = 1, \dots, M.$$

In other words, for each of the  $M$  random variables  $\xi_1, \dots, \xi_M$  we seek a set of polynomials  $\{\widehat{\psi}_j^{(m)}\}_{j=0}^p$  of degree  $p$  with the properties

$$\langle \widehat{\psi}_i^{(m)} \widehat{\psi}_j^{(m)} \rangle = \int_{\Gamma_m} \widehat{\psi}_i^{(m)}(\xi) \widehat{\psi}_j^{(m)}(\xi) \rho_m(\xi) d\xi = \delta_{i,j}, \quad (3.4a)$$

$$\langle \xi \widehat{\psi}_i^{(m)} \widehat{\psi}_j^{(m)} \rangle = \int_{\Gamma_m} \widehat{\psi}_i^{(m)}(\xi) \widehat{\psi}_j^{(m)}(\xi) \xi \rho_m(\xi) d\xi = \delta_{i,j} \lambda_i^{(m)}, \quad (3.4b)$$

for  $i, j = 0, \dots, p$  and  $m = 1, \dots, M$ . In [5] Babuška et al. suggested the name *double-orthogonal polynomials* for polynomials satisfying (3.4), since they are simultaneously orthogonal with respect to the ‘weight functions’  $w(\xi) = \rho_m(\xi)$  and  $w(\xi) = \xi \rho_m(\xi)$ .

To compute such double-orthogonal polynomials in general an immediate approach is to represent the polynomials with respect to the monomial basis  $\{1, \xi, \dots, \xi^p\}$  such that (dropping the superscripts and subscripts referring to  $m$  for now)

$$[\widehat{\psi}_0, \widehat{\psi}_1, \dots, \widehat{\psi}_p] = [1, \xi, \dots, \xi^p] V$$

Inserting this representation into (3.4) reveals that  $V$  is the solution of the generalized eigenvalue problem

$$M_1 V = M_0 V \Lambda$$

in terms of the moment matrices

$$[M_0]_{i,j} = \langle \xi^{i+j} \rangle, \quad [M_1]_{i,j} = \langle \xi^{i+j+1} \rangle, \quad i, j = 0, 1, \dots, p.$$

A simpler (standard) eigenvalue problem is obtained if we start from the basis of orthonormal polynomials  $\{\psi_j\}_{j=0}^p$  instead of the monomials. In this case the moment matrix is replaced with the Gramian matrix of this basis, i.e., the identity, and the matrix  $M_1$  is replaced by the matrix

$$U_1 = [\langle \xi \psi_i(\xi) \psi_j(\xi) \rangle]_{i,j=0}^p,$$

which we identified in (2.17) as the symmetric tridiagonal *Jacobi matrix* associated with the weight function  $\rho$ .

In summary, constructing the double-orthogonal polynomial basis  $\widehat{\Psi}$  of  $\mathcal{V}_p$  requires only the Jacobi matrices  $U_1^{(m)}$  up to degree  $p$  for each of the probability density functions  $\rho_m$ ,  $m = 1, 2, \dots, M$  or, equivalently, the coefficients  $\{\alpha_j, \beta_j\}_{j=0}^p$  for the three-term recurrence of the orthogonal polynomials generated by  $\rho_m$ . These can be either obtained from the literature or generated using the well-known Stieltjes procedure, the polynomial equivalent of the Lanczos process. The columns of the matrices  $V_m$  in (3.2) and (3.3) are then obtained as the normalized eigenvectors of the Jacobi matrices  $U_1^{(m)}$  with the corresponding eigenvalues forming the diagonal of the matrices  $\Lambda_m$  in (3.3).

**THEOREM 5.** *For the space of tensor product polynomials  $\mathcal{V}_p$  the Stochastic Galerkin matrices  $\{\mathbf{G}_m\}_{m=0}^M$  are simultaneously diagonalized by the Hermitian matrix  $\mathbf{V} = V_M \otimes V_{M-1} \otimes \dots \otimes V_1$  in (3.2), the Kronecker factors of which contain the orthonormal eigenvectors of the univariate matrices  $U_1^{(m)}$ , resulting in the  $M$  diagonal matrices*

$$\widehat{\mathbf{G}}_m = \mathbf{V}^\top \mathbf{G}_m \mathbf{V} = I_{p+1} \otimes \dots \otimes I_{p+1} \otimes \Lambda_m \otimes I_{p+1} \otimes \dots \otimes I_{p+1}, \quad m = 1, 2, \dots, M,$$

as well as  $\widehat{\mathbf{G}}_0 = \mathbf{I}$ . The diagonal matrices  $\Lambda_m$  contain the eigenvalues of the matrices  $U_1^{(m)}$ , respectively, i.e., the zeros of the orthogonal polynomial of degree  $p+1$  associated with the weight function  $\rho_m$ . The matrix  $\mathbf{V}$  effects a change of basis from the orthogonal polynomials  $\{\psi_j\}_{j=0}^p$  to the basis of double-orthogonal polynomials  $\{\widehat{\psi}_j\}_{j=0}^p$  satisfying (3.4).

We note that the same argument applies also when different polynomial degrees  $p_m$  are used in each random variable and emphasize that each random variable may have a different probability density  $\rho_m$ . Moreover, the distributions need not possess a density function, all that is needed is the recurrence coefficients  $\{\alpha_j^{(m)}, \beta_j^{(m)}\}_{j=0}^p$ , i.e., the existence of the distribution's moments. What is crucial to the diagonalization is the tensor product structure of the polynomial space, which is a direct consequence of the independence of the random variables  $\xi_m$ .

**3.2. Complete polynomials.** Turning now to the space  $\mathcal{V}_p^C$  of complete polynomials, we assume  $M > 1$  and  $p > 0$  to avoid trivial cases.

**LEMMA 6.** *For the stochastically linear case with  $M > 1$  random variables and polynomial degree  $p \geq 1$ , the Stochastic Galerkin matrices  $\{\mathbf{G}_m^C\}_{m=1}^M$  associated with the space of complete polynomials  $\mathcal{V}_p^C$  are singular.*

*Proof.* For each of the matrices  $\{\mathbf{G}_m^C\}_{m=1}^M$ , we find a nonzero basis function which is mapped to zero by the operator represented by  $\mathbf{G}_m^C$ .

For each fixed  $m$ , our assumptions  $M > 1$  and  $p > 0$  imply that the polynomial basis  $\Psi$  in (2.8) contains at least one polynomial

$$\psi(\boldsymbol{\xi}) = \psi_p^{(k)}(\xi_k), \quad k \neq m,$$

of exact degree  $p$  depending only on the  $k$ -th random variable  $\xi_k$ . When applied to  $\psi$ , the multiplication operator associated with  $\mathbf{G}_m^C$  yields the orthogonal projection of the polynomial  $\xi_m \psi(\boldsymbol{\xi})$  onto  $\mathcal{V}_p^C$ . We verify that  $\xi_m \psi(\boldsymbol{\xi})$  is orthogonal to  $\mathcal{V}_p^C$ . Indeed, for any basis polynomial  $\psi_\alpha$ ,  $\alpha \in \mathcal{I}_p^C$ , we obtain

$$\langle \xi_m \psi(\boldsymbol{\xi}) \psi_\alpha(\boldsymbol{\xi}) \rangle = \left\langle \xi_m \psi_p^{(k)}(\xi_k) \prod_{\ell=1}^M \psi_{\alpha_\ell}^{(\ell)}(\xi_\ell) \right\rangle = \langle \xi_m \psi_{\alpha_m}^{(m)}(\xi_m) \rangle \langle \psi_p^{(k)}(\xi_k) \psi_{\alpha_k}^{(k)}(\xi_k) \rangle \prod_{\substack{\ell=1 \\ \ell \neq m, k}}^M \langle \psi_{\alpha_\ell}^{(\ell)}(\xi_\ell) \rangle$$

and assert that one of the first two factors on the right of the last equality must vanish. Otherwise, a nonzero first factor implies  $\alpha_m = 1$  and for the second factor not to vanish it is necessary that  $\alpha_k = p$ , which together imply  $|\alpha| \geq p + 1$ , a contradiction to  $\psi_\alpha \in \mathcal{V}_p^C$ .  $\square$

**THEOREM 7.** *For the stochastically linear case with  $M > 1$  random variables and polynomial degree  $p \geq 1$ , the Stochastic Galerkin matrices  $\{\mathbf{G}_m^C\}_{m=0}^M$  associated with the space of complete polynomials  $\mathcal{V}_p^C$  are not simultaneously diagonalizable.*

*Proof.* In the proof of Lemma 6 it was shown that for each matrix  $\mathbf{G}_m^C$  there exists an index  $k \neq m$  such that  $\psi_p^{(k)}$  lies in the nullspace of the operator represented by  $\mathbf{G}_m^C$ , i.e.,  $\psi_p^{(k)}$  is an eigenfunction associated with eigenvalue zero. We show that this polynomial is not an eigenfunction of the operator represented by  $\mathbf{G}_k^C$ , a necessary condition for simultaneous diagonalizability.

Otherwise, we would have

$$\left\langle \xi_k \psi_p^{(k)}(\xi_k) \psi_\alpha(\boldsymbol{\xi}) \right\rangle = \lambda \left\langle \psi_p^{(k)}(\xi_k) \psi_\alpha(\boldsymbol{\xi}) \right\rangle, \quad \forall \psi_\alpha \in \Psi.$$

In particular, choosing  $\psi_\alpha = \psi_{p-1}^{(k)}$ , we obtain

$$\left\langle \xi_k \psi_p^{(k)}(\xi_k) \psi_{p-1}^{(k)}(\xi_k) \right\rangle = \lambda \left\langle \psi_p^{(k)}(\xi_k) \psi_{p-1}^{(k)}(\xi_k) \right\rangle = 0$$

by orthogonality of  $\psi_{p-1}^{(k)}$  and  $\psi_p^{(k)}$ . The term on the left, however, is just the last entry on the first subdiagonal of the Jacobi matrix  $U_1^{(k)}$  associated with the orthonormal polynomials generated by the weight function  $\rho_k$ . Since this quantity is always positive (see [11, Definition 1.30 and Theorem 1.27]), we have arrived at a contradiction.  $\square$

Many authors use the space of complete polynomials  $\mathcal{V}_p$  for the stochastic discretization, see e.g. [13, 19, 22, 21], to avoid the so-called ‘curse of dimensionality’ since the number of degrees of freedom in  $\mathcal{V}_p$  grows exponentially with the number of random variables  $M$  in contrast to  $\mathcal{V}_p^C$  where this growth is only algebraic (cf. (2.3)). On the other hand, Theorem 7 shows that an uncoupling of the equations is not possible for this smaller space. By consequence, in stochastic Galerkin discretizations of coupled deterministic-stochastic problems, using the smaller space of complete polynomials of degree  $p$  requires the solution of large linear systems of equations in which several instances of the deterministic problem are coupled, see [12, 20, 21, 10, 8] for methods for solving the fully coupled system.

**4. Eigenvalues of Stochastic Galerkin matrices.** In this section we present eigenvalue location results for Stochastic Galerkin matrices. Such results, besides being of interest in their own right, are necessary in the analysis of preconditioning schemes for Stochastic Galerkin discretizations (cf. [21, 10, 8]).

**4.1. Tensor product polynomials.** We begin with the simpler situation of tensor product polynomials. The Kronecker product structure of the Stochastic Galerkin matrices in this case immediately yields the following eigenvalue bounds.

**THEOREM 8.** *The eigenvalues of the Stochastic Galerkin matrices  $\mathbf{G}_\alpha$  for the space  $\mathcal{V}_p$  of tensor product polynomials are given by*

$$\Lambda(\mathbf{G}_\alpha) = \left\{ \prod_{m=1}^M \lambda^{(m)} : \lambda^{(m)} \in \Lambda(U_{\alpha_m}^{(m)}) \right\}, \quad \alpha = (\alpha_1, \dots, \alpha_M) \in \mathcal{I}_p. \quad (4.1)$$

*Proof.* (4.1) follows from the well-known expression for the eigenvalues of a Kronecker product (2.11), as can be found e.g. in [15, Theorem 4.2.12].  $\square$

COROLLARY 9. *In the stochastically linear case the eigenvalues of the Stochastic Galerkin matrices  $\{\mathbf{G}_m\}_{m=1}^M$  obtained for the space of tensor product polynomials  $\mathcal{V}_p$  are given by*

$$\Lambda(\mathbf{G}_m) = \Lambda(U_1^{(m)}), \quad m = 1, \dots, M.$$

*In other words, the eigenvalues consist of the roots of the orthogonal polynomial of degree  $p + 1$  generated by the weight function  $\rho_m$ .*

*Proof.* This follows immediately from (2.12) and the discussion at the end of Section 2.  $\square$

In the stochastically nonlinear case, a complete characterization of the eigenvalues of the matrices  $\mathbf{G}_\alpha$  requires the eigenvalues of the matrices  $U_n^{(m)}$  associated with the univariate weight function  $\rho_m$  for  $n \geq 2$ . Some first results on this topic are presented in Section 4.4. In general, however, the complete information on the eigenvalues of these matrices is not available. We therefore show how inclusion bounds on the spectrum of the Stochastic Galerkin matrices may be obtained with the help of suitable Gaussian quadrature rules.

To this end, let  $(\eta_{m,i}, w_{m,i})_{i=1}^{\delta_m}$  denote the nodes and weights, respectively, of the  $\delta_m$ -point Gaussian quadrature rule associated with the probability density function  $\rho_m$ ,  $m = 1, \dots, M$ . That is,

$$\langle \psi \rangle = \int_{\Gamma_m} \psi(\xi) \rho_m(\xi) d\xi \approx \sum_{i=1}^{\delta_m} \psi^{(m)}(\eta_{m,i}) w_{m,i}.$$

Each quadrature rule above is exact for polynomials  $\psi \in \text{span}\{1, \xi, \dots, \xi^{2\delta_m-1}\}$ . Furthermore, we define the tensor product grid of quadrature nodes,

$$\Xi_\delta := \bigtimes_{m=1}^M \{\eta_{m,1}, \eta_{m,2}, \dots, \eta_{m,\delta_m}\}, \quad (4.2)$$

in which the components  $\delta_m$  of the multi-index  $\delta \in \mathbb{N}_0^M$  denote the number of nodes in the  $m$ -th quadrature rule.

THEOREM 10. *The eigenvalues of the Stochastic Galerkin matrices  $\mathbf{G}_\alpha$  for the space  $\mathcal{V}_p$  of tensor product polynomials with the basis  $\{\psi_\alpha\}$  introduced in (2.8) are bounded by  $\Lambda(\mathbf{G}_\alpha) \subset [\theta_\alpha, \Theta_\alpha]$ , where*

$$\theta_\alpha := \min\{\psi_\alpha(\boldsymbol{\eta}) : \boldsymbol{\eta} \in \Xi_\delta\}, \quad \Theta_\alpha := \max\{\psi_\alpha(\boldsymbol{\eta}) : \boldsymbol{\eta} \in \Xi_\delta\}, \quad \alpha \in \mathcal{I}_{2p}, \quad (4.3)$$

where  $\Xi_\delta$  is an  $M$ -dimensional grid of quadrature nodes as defined in (4.2), in which the number of nodes in the  $m$ -th rule is at least  $\delta_m := p + \lceil \frac{\alpha_m + 1}{2} \rceil$ ,  $m = 1, \dots, M$ .

*Proof.* Since the Stochastic Galerkin matrices  $\mathbf{G}_\alpha$ ,  $\alpha \in \mathcal{I}_{2p}$ , are symmetric, the largest eigenvalue of  $\mathbf{G}_\alpha$  satisfies:

$$\begin{aligned} \lambda_{\max}(\mathbf{G}_\alpha) &= \max_{\mathbf{v} \in \mathbb{R}^{N_p} \setminus \{0\}} \frac{\mathbf{v}^\top \mathbf{G}_\alpha \mathbf{v}}{\mathbf{v}^\top \mathbf{v}} = \max_{\psi \in \mathcal{V}_p \setminus \{0\}} \frac{\langle \psi_\alpha \psi^2 \rangle}{\langle \psi^2 \rangle} = \max \frac{\sum_{\beta, \gamma \in \mathcal{I}_p} c_\beta c_\gamma \langle \psi_\alpha \psi_\beta \psi_\gamma \rangle}{\sum_{\beta, \gamma \in \mathcal{I}_p} c_\beta c_\gamma \langle \psi_\beta \psi_\gamma \rangle} \\ &= \max \frac{\sum_{\beta, \gamma \in \mathcal{I}_p} c_\beta c_\gamma \prod_{m=1}^M \sum_{i=1}^{\delta_m} \psi_{\alpha_m}^{(m)}(\eta_{m,i}) \psi_{\beta_m}^{(m)}(\eta_{m,i}) \psi_{\gamma_m}^{(m)}(\eta_{m,i}) w_{m,i}}{\sum_{\beta, \gamma \in \mathcal{I}_p} c_\beta c_\gamma \prod_{m=1}^M \sum_{i=1}^{\delta_m} \psi_{\beta_m}^{(m)}(\eta_{m,i}) \psi_{\gamma_m}^{(m)}(\eta_{m,i}) w_{m,i}} \end{aligned}$$

for  $2\delta_m - 1 \geq \alpha_m + 2p$ , or, equivalently,  $\delta_m \geq p + \lceil \frac{\alpha_m + 1}{2} \rceil$ ,  $m = 1, \dots, M$ . In addition, the numerator in the last expression above can be estimated as follows,

$$\begin{aligned} &\sum_{\beta, \gamma \in \mathcal{I}_p} c_\beta c_\gamma \prod_{m=1}^M \sum_{i=1}^{\delta_m} \psi_{\alpha_m}^{(m)}(\eta_{m,i}) \psi_{\beta_m}^{(m)}(\eta_{m,i}) \psi_{\gamma_m}^{(m)}(\eta_{m,i}) w_{m,i} \\ &\leq \max \left\{ \prod_{m=1}^M \psi_{\alpha_m}^{(m)}(\eta_{m,i}) : i = 1, \dots, \delta_m, m = 1, \dots, M \right\} \\ &\quad \sum_{\beta, \gamma \in \mathcal{I}_p} c_\beta c_\gamma \prod_{m=1}^M \sum_{i=1}^{\delta_m} \psi_{\beta_m}^{(m)}(\eta_{m,i}) \psi_{\gamma_m}^{(m)}(\eta_{m,i}) w_{m,i}. \end{aligned}$$

Thus, defining the multi-index  $\delta \in \mathbb{N}_0^M$  with  $\delta_m := p + \lceil \frac{\alpha_m + 1}{2} \rceil$ ,  $m = 1, \dots, M$ , we obtain the desired result for the largest eigenvalue of  $\mathbf{G}_\alpha$ :

$$\lambda_{\max}(\mathbf{G}_\alpha) \leq \max \left\{ \prod_{m=1}^M \psi_{\alpha_m}^{(m)}(\eta_{m,i}) : i = 1, \dots, \delta_m, m = 1, \dots, M \right\} = \max \{ \psi_\alpha(\boldsymbol{\eta}) : \boldsymbol{\eta} \in \Xi_\delta \}.$$

The lower bound for the smallest eigenvalue of  $\mathbf{G}_\alpha$  follows analogously.  $\square$

**COROLLARY 11.** *In the stochastically linear case, the inclusion bound in (4.3) is sharp.*

*Proof.* For  $|\alpha| = 1$ ,  $\alpha_m = 1$ , we have  $\delta_m = p + 1$ ,  $m = 1, \dots, M$ , in Theorem 10. Noting that  $\psi_\alpha(\boldsymbol{\xi}) = \psi^{(m)}(\xi_m) = \xi_m$ , the spectral bounds for  $\mathbf{G}_\alpha$  in (4.3) read

$$\theta_\alpha = \min_{i=1, \dots, p+1} \{ \eta_{m,i} \}, \quad \Theta_\alpha = \max_{i=1, \dots, p+1} \{ \eta_{m,i} \}.$$

Finally, since the quadrature nodes  $\eta_{m,i}$ ,  $i = 1, \dots, p + 1$ , are the zeros of  $\psi_{p+1}^{(m)}$ , the assertion follows from Corollary 9.  $\square$

**4.2. Complete polynomials.** For the complete polynomial spaces  $\mathcal{V}_p^C$  the eigenvalues of the associated Stochastic Galerkin matrices  $\mathbf{G}_\alpha^C$  may be bounded by those of their tensor product polynomial counterparts.

**COROLLARY 12.** *The eigenvalues of the Stochastic Galerkin matrices  $\mathbf{G}_\alpha^C$  for the space  $\mathcal{V}_p^C$  of complete polynomials are bounded by*

$$\Lambda(\mathbf{G}_\alpha^C) \subset [\lambda_{\min}(\mathbf{G}_\alpha), \lambda_{\max}(\mathbf{G}_\alpha)], \quad \alpha \in \mathcal{I}_{2p}^C, \quad (4.4)$$

where for each multi-index  $\alpha \in \mathcal{I}_{2p}^C$  the matrix  $\mathbf{G}_\alpha = [\langle \psi_\alpha \psi_\beta \psi_\gamma \rangle]_{\beta, \gamma \in \mathcal{I}_p}$  denotes the stochastic Galerkin matrix with the same multi-index  $\alpha$  where the polynomials  $\psi_\beta$  and  $\psi_\gamma$  vary over  $\mathcal{V}_p$  rather than the smaller space  $\mathcal{V}_p^C$ .

*Proof.* The inclusion (4.4) follows by a Rayleigh quotient argument because for each  $\alpha \in \mathcal{I}_{2p}^C$  the matrix  $\mathbf{G}_\alpha^C$  is a principal submatrix of  $\mathbf{G}_\alpha$  (see [14, Theorem 4.3.15]).  $\square$

**COROLLARY 13.** *The eigenvalues of the Stochastic Galerkin matrices  $\mathbf{G}_\alpha^C$  for the space  $\mathcal{V}_p^C$  of complete polynomials are bounded by*

$$\Lambda(\mathbf{G}_\alpha^C) \subset [\theta_\alpha, \Theta_\alpha], \quad \alpha \in \mathcal{I}_{2p}^C,$$

where  $\theta_\alpha$  and  $\Theta_\alpha$  are defined in (4.3).

*Proof.* This follows from Corollary 12 and Theorem 10.  $\square$

In the stochastically linear case for complete polynomials we can characterize the eigenvalues completely. (See also [21, Lemma 3.1] for the same observation in a more restricted context.)

**THEOREM 14.** *In the stochastically linear case the eigenvalues of the Stochastic Galerkin matrices  $\{\mathbf{G}_m^C\}_{m=1}^M$  for the space  $\mathcal{V}_p^C$  of complete polynomials are given by*

$$\Lambda(\mathbf{G}_m^C) = \bigcup_{j=1}^{p+1} \Lambda(U_{1,j}^{(m)}), \quad (4.5)$$

where  $U_{1,j}^{(m)}$  denotes the  $j$ -th leading principal submatrix of the Jacobi matrix  $U_1^{(m)} \in \mathbb{R}^{(p+1) \times (p+1)}$  associated with the weight function  $\rho_m$ . In other words, the eigenvalues of  $\mathbf{G}_m^C$  consist of the union of all zeros of the orthonormal polynomials  $\{\psi_j^{(m)}\}_{j=1}^{p+1}$  generated by the weight function  $\rho_m$ .

*Proof.* This assertion follows from the fact that, as shown in the proof of Lemma 3, the matrices  $\mathbf{G}_m^C$  are permutation-similar to a block diagonal matrix whose diagonal blocks are Jacobi matrices of dimension  $1, 2, \dots, p + 1$  associated with the orthonormal polynomials generated by the weight function  $\rho_m$ , where all Jacobi matrices occur.  $\square$

**COROLLARY 15.** *In the stochastically linear case the inclusion bound (4.4) is sharp.*

*Proof.* This follows from Theorem 14 and the interlacing property of the zeros of real orthogonal polynomials (cf. [11, Theorem 1.20]).  $\square$



**4.3. Even weight functions and the multivariate case.** We shall assume throughout the remainder of this section that the weight functions  $\rho_m$  and therefore also their product are even functions of  $\boldsymbol{\xi}$ , i.e., that

$$\rho_m(-\xi_m) = \rho_m(\xi_m) \quad \forall \xi_m \in \Gamma_m. \quad (4.6)$$

In the primary case of interest where the weight functions  $\rho_m$  are probability density functions, (4.6) is satisfied for many commonly occurring probability distributions, notably the centered Gaussian distribution as well as a centered uniform distribution.

**PROPOSITION 16.** *For even weight functions the associated multivariate orthonormal basis polynomials  $\psi_\alpha$  in (2.8) are even or odd functions according to whether their total degree  $|\alpha|$  is even or odd, respectively, i.e., there holds*

$$\psi_\alpha(\boldsymbol{\xi}) = (-1)^{|\alpha|} \psi_\alpha(-\boldsymbol{\xi}) \quad \forall \alpha \in \mathbb{N}_0^M. \quad (4.7)$$

*Proof.* In [11, Theorem 1.17] this relation is established for monic univariate orthogonal polynomials. After normalization we have

$$\psi_j^{(m)}(\xi_m) = (-1)^j \psi_j^{(m)}(-\xi_m), \quad j \geq 0, \quad m = 1, \dots, M.$$

Hence for the multivariate orthonormal polynomials in (2.8) we obtain

$$\psi_\alpha(\boldsymbol{\xi}) = \prod_{m=1}^M \psi_{\alpha_m}^{(m)}(\xi_m) = \prod_{m=1}^M (-1)^{\alpha_m} \psi_{\alpha_m}^{(m)}(-\xi_m) = (-1)^{|\alpha|} \psi_\alpha(-\boldsymbol{\xi}).$$

□

**PROPOSITION 17.** *For even weight functions the entries of the Stochastic Galerkin matrices  $\mathbf{G}_\alpha$  satisfy the relation*

$$\langle \psi_\alpha \psi_\beta \psi_\gamma \rangle = (-1)^{|\alpha|+|\beta|+|\gamma|} \langle \psi_\alpha \psi_\beta \psi_\gamma \rangle. \quad (4.8)$$

*Proof.* Relation (4.8) follows from (4.7) by substituting  $-\xi_m$  for  $\xi_m$  in the  $M$  integrals into which  $\langle \psi_\alpha \psi_\beta \psi_\gamma \rangle$  decouples. □

For multi-indices  $\alpha$  of odd degree the symmetry property (4.7) of the basis polynomials results in a symmetric spectrum for  $\mathbf{G}_\alpha$ .

**THEOREM 18.** *For even weight functions the eigenvalues of the Stochastic Galerkin matrices  $\mathbf{G}_\alpha$  lie symmetric with respect to the origin.*

*Proof.* To show that  $\lambda \in \Lambda(\mathbf{G}_\alpha)$  implies  $-\lambda \in \Lambda(\mathbf{G}_\alpha)$  denote by  $[\mathbf{v}]_\beta$ ,  $\beta \in \mathcal{I}$ , where  $\mathcal{I}$  denotes either  $\mathcal{I}_p$  or  $\mathcal{I}_p^C$ , the components of the eigenvector  $\mathbf{v}$  associated with an eigenvalue  $\lambda$ . Setting  $\tilde{\mathbf{v}}$  to be the vector obtained by replacing the component  $[\mathbf{v}]_\beta$  of  $\mathbf{v}$  with  $(-1)^{|\beta|} [\mathbf{v}]_\beta$ , there holds

$$\begin{aligned} [\mathbf{G}_\alpha \tilde{\mathbf{v}}]_\beta &= \sum_{\gamma \in \mathcal{I}} \langle \psi_\alpha \psi_\beta \psi_\gamma \rangle [\tilde{\mathbf{v}}]_\gamma = \sum_{\gamma \in \mathcal{I}} (-1)^{|\alpha|+|\beta|+|\gamma|} \langle \psi_\alpha \psi_\beta \psi_\gamma \rangle (-1)^{|\gamma|} [\mathbf{v}]_\gamma \\ &= (-1)^{|\alpha|+|\beta|} \lambda [\mathbf{v}]_\beta = -\lambda [\tilde{\mathbf{v}}]_\beta. \end{aligned}$$

□

**4.4. Even weight functions and the univariate case.** In the remainder of this section we present some first results on the eigenvalues of the Stochastic Galerkin matrices in the univariate case, i.e., the matrices  $U_n^{(m)}$ . For clarity of presentation we omit the superscript  $(m)$ . Note that, for typographical reasons, we shall represent finite sequences of orthogonal polynomials as *column vectors* in this section. Since all matrices of recurrence coefficients are symmetric this should not cause confusion.

We first recall that for even weight functions the diagonal recurrence coefficients  $\alpha_k$  in (2.16) and (2.17) vanish, i.e., the three-term recurrence (2.16) simplifies to

$$\sqrt{\beta_{k+1}}\psi_{k+1}(\xi) = \xi\psi_k(\xi) - \sqrt{\beta_k}\psi_{k-1}(\xi), \quad k = 0, 1, \dots, \quad \psi_{-1} \equiv 0, \quad (4.9)$$

and the associated tridiagonal Jacobi matrices  $U_1$  have a vanishing diagonal.

The connection of eigenvalues of the matrices  $U_1 =: U_{1,p} \in \mathbb{R}^{(p+1) \times (p+1)}$  to the zeros of  $\psi_{p+1}$  is revealed by collecting the recurrence relations (4.9) for  $k = 0, 1, \dots, p$ , yielding

$$\xi \begin{bmatrix} \psi_0(\xi) \\ \psi_1(\xi) \\ \vdots \\ \psi_{p-1}(\xi) \\ \psi_p(\xi) \end{bmatrix} = U_{1,p} \begin{bmatrix} \psi_0(\xi) \\ \psi_1(\xi) \\ \vdots \\ \psi_{p-1}(\xi) \\ \psi_p(\xi) \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \sqrt{\beta_{p+1}}\psi_{p+1}(\xi) \end{bmatrix}. \quad (4.10)$$

For each of the  $p+1$  distinct zeros  $\{\mu_{p+1,\ell}\}_{\ell=1}^{p+1}$  of  $\psi_{p+1}$ , setting  $\xi = \mu_{p+1,\ell}$  in (4.10) represents an eigenvalue-eigenvector relation for the matrix  $U_{1,p}$ .

To determine the eigenvalues of the matrices  $U_{2,p}$  we first establish a recurrence relation similar to (4.9) for the product  $\psi_2\psi_k$ .

LEMMA 19. *For even weight functions the polynomial sequence  $\{\psi_2\psi_k\}_{k \geq 0}$  satisfies the five-term recurrence*

$$\psi_2\psi_k = c_2\sqrt{\beta_{k+2}\beta_{k+1}}\psi_{k+2} + [c_2(\beta_{k+1} + \beta_k) + c_0]\psi_k + c_2\sqrt{\beta_k\beta_{k-1}}\psi_{k-2}, \quad k = 0, 1, 2, \dots, \quad (4.11)$$

where  $\psi_2(\xi) = c_2\xi^2 + c_0$ , and  $\psi_k(\xi) \equiv 0$  for  $k = -1, -2$ .

*Proof.* Recalling from the proof of Proposition 16 that the orthonormal polynomial  $\psi_2$  is an even function, we may factor it as

$$\psi_2(\xi) = c_2(\xi - \lambda)(\xi + \lambda), \quad (4.12)$$

where  $\lambda$  denotes the positive root. From the recurrence relation (4.9) we deduce

$$(\xi + \lambda)\psi_k(\xi) = \sqrt{\beta_{k+1}}\psi_{k+1}(\xi) + \lambda\psi_k(\xi) + \sqrt{\beta_k}\psi_{k-1}(\xi), \quad (4.13)$$

$$(\xi - \lambda)\psi_k(\xi) = \sqrt{\beta_{k+1}}\psi_{k+1}(\xi) - \lambda\psi_k(\xi) + \sqrt{\beta_k}\psi_{k-1}(\xi). \quad (4.14)$$

Utilizing (4.12) together with (4.13) and (4.14) we obtain

$$\begin{aligned} \psi_2(\xi)\psi_k(\xi) &= c_2(\xi - \lambda)(\xi + \lambda)\psi_k(\xi) \\ &= c_2(\xi - \lambda) \left( \sqrt{\beta_{k+1}}\psi_{k+1}(\xi) + \lambda\psi_k(\xi) + \sqrt{\beta_k}\psi_{k-1}(\xi) \right) \\ &= c_2\sqrt{\beta_{k+1}} \left( \sqrt{\beta_{k+2}}\psi_{k+2}(\xi) - \lambda\psi_{k+1}(\xi) + \sqrt{\beta_{k+1}}\psi_k(\xi) \right) \\ &\quad + c_2\lambda \left( \sqrt{\beta_{k+1}}\psi_{k+1}(\xi) - \lambda\psi_k(\xi) + \sqrt{\beta_k}\psi_{k-1}(\xi) \right) \\ &\quad + c_2\sqrt{\beta_k} \left( \sqrt{\beta_k}\psi_k(\xi) - \lambda\psi_{k-1}(\xi) + \sqrt{\beta_{k-1}}\psi_{k-2}(\xi) \right) \\ &= c_2\sqrt{\beta_{k+2}\beta_{k+1}}\psi_{k+2}(\xi) + c_2(\beta_{k+1} + \beta_k - \lambda^2)\psi_k(\xi) + c_2\sqrt{\beta_k\beta_{k-1}}\psi_{k-2}(\xi). \end{aligned}$$

Substituting  $c_0 = \psi_2(0) = -c_2\lambda^2$  establishes (4.11).  $\square$

Collecting the five-term recurrence (4.11) for  $k = 0, 1, \dots, p$  in a manner analogous to (4.10) now yields

$$\psi_2(\xi) \begin{bmatrix} \psi_0(\xi) \\ \psi_1(\xi) \\ \vdots \\ \psi_{p-1}(\xi) \\ \psi_p(\xi) \end{bmatrix} = U_{2,p} \begin{bmatrix} \psi_0(\xi) \\ \psi_1(\xi) \\ \vdots \\ \psi_{p-1}(\xi) \\ \psi_p(\xi) \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ c_2\sqrt{\beta_{p+1}\beta_p}\psi_{p+1}(\xi) \\ c_2\sqrt{\beta_{p+2}\beta_{p+1}}\psi_{p+2}(\xi) \end{bmatrix}.$$

To obtain an eigenvalue-eigenvector relation it is necessary that both the last two entries vanish in the last vector on the right for some values of  $\xi$ . By the interlacing property of real orthogonal polynomials, however, it follows that  $\psi_{p+1}$  and  $\psi_{p+2}$  have no common zeros. However, if the basis polynomials are ordered in an odd-even fashion, i.e.,

$$\psi_0(\xi), \psi_2(\xi), \psi_4(\xi), \dots, \psi_p(\xi), \psi_1(\xi), \psi_3(\xi), \dots, \psi_{p-1}(\xi),$$

assuming  $p$  is even, the following block  $2 \times 2$  structure emerges:

$$\psi_2(\xi) \begin{bmatrix} \psi_0(\xi) \\ \psi_2(\xi) \\ \vdots \\ \psi_p(\xi) \\ \psi_1(\xi) \\ \psi_3(\xi) \\ \vdots \\ \psi_{p-1}(\xi) \end{bmatrix} = \begin{bmatrix} U_{2,p}^{\text{even}} & O \\ O & U_{2,p}^{\text{odd}} \end{bmatrix} \begin{bmatrix} \psi_0(\xi) \\ \psi_2(\xi) \\ \vdots \\ \psi_p(\xi) \\ \psi_1(\xi) \\ \psi_3(\xi) \\ \vdots \\ \psi_{p-1}(\xi) \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ c_2\sqrt{\beta_{p+2}\beta_{p+1}}\psi_{p+2}(\xi) \\ 0 \\ \vdots \\ 0 \\ c_2\sqrt{\beta_{p+1}\beta_p}\psi_{p+1}(\xi) \end{bmatrix}. \quad (4.15)$$

The reordered matrix  $U_{2,p}$  is block diagonal because the recurrence (4.11) only couples polynomials of even index with polynomials with even index, as well as odd with odd, respectively. The block diagonal structure in (4.15) now reveals that the eigenvalues of  $U_{2,p}$  are those of  $U_{2,p}^{\text{even}}$  together with those of  $U_{2,p}^{\text{odd}}$ . These are obtained by considering the two uncoupled recurrences

$$\psi_2(\xi) \begin{bmatrix} \psi_0(\xi) \\ \psi_2(\xi) \\ \vdots \\ \psi_p(\xi) \end{bmatrix} = U_{2,p}^{\text{even}} \begin{bmatrix} \psi_0(\xi) \\ \psi_2(\xi) \\ \vdots \\ \psi_p(\xi) \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ c_2\sqrt{\beta_{p+2}\beta_{p+1}}\psi_{p+2}(\xi) \end{bmatrix}$$

and

$$\psi_2(\xi) \begin{bmatrix} \psi_1(\xi) \\ \psi_3(\xi) \\ \vdots \\ \psi_{p-1}(\xi) \end{bmatrix} = U_{2,p}^{\text{odd}} \begin{bmatrix} \psi_1(\xi) \\ \psi_3(\xi) \\ \vdots \\ \psi_{p-1}(\xi) \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ c_2\sqrt{\beta_{p+1}\beta_p}\psi_{p+1}(\xi) \end{bmatrix}.$$

Turning to the first, we observe that  $\psi_{p+2}$  has  $p+2$  roots which lie symmetrically about the origin. In view of the fact that  $\psi_2(\xi)$  is an even function of  $\xi$ , we conclude that all eigenvalues of  $U_{2,p}^{\text{even}}$  are obtained by inserting the positive roots of  $\psi_{p+2}$  into  $\psi_2$ . Analogously, in the odd recurrences we obtain the eigenvalues of  $U_{2,p}^{\text{odd}}$  by inserting the positive roots of  $\psi_{p+1}$  into  $\psi_2$ .

Noting that the case of  $p$  odd works in an analogous manner, we summarize our findings in THEOREM 20.

(a) In case  $p = 2k$ ,  $k \in \mathbb{N}_0$ , assuming even weight functions, the eigenvalues of the univariate stochastic Galerkin matrix  $U_{2,p}$  are given by

$$\Lambda(U_{2,p}) = \{\psi_2(\mu_{p+2,\ell})\}_{\ell=1}^{k+1} \cup \{\psi_2(\mu_{p+1,\ell})\}_{\ell=1}^k,$$

where  $\{\mu_{p+2,\ell}\}_{\ell=1}^{k+1}$  denote the  $k+1$  positive roots of  $\psi_{p+2}$  and  $\{\mu_{p+1,\ell}\}_{\ell=1}^k$  denote the  $k$  positive roots of  $\psi_{p+1}$ .

(b) In case  $p = 2k+1$ ,  $k \in \mathbb{N}_0$ , assuming even weight functions, the eigenvalues of  $U_{2,p}$  are given by

$$\Lambda(U_{2,p}) = \{\psi_2(\mu_{p+2,\ell})\}_{\ell=1}^{k+1} \cup \{\psi_2(\mu_{p+1,\ell})\}_{\ell=1}^{k+1},$$

where  $\{\mu_{p+2,\ell}\}_{\ell=1}^{k+1}$  denote the  $k+1$  positive roots of  $\psi_{p+2}$  and  $\{\mu_{p+1,\ell}\}_{\ell=1}^{k+1}$  denote the  $k+1$  positive roots of  $\psi_{p+1}$ .

COROLLARY 21. Assuming even weight functions, the upper inclusion bound in (4.3) for the univariate stochastic Galerkin matrix  $U_{2,p}$  is sharp.

*Proof.* For  $M = 1$  and  $\alpha = (2)$  we have  $\delta = (p+2)$  in Theorem 10. Thus, for the matrix  $U_{2,p}$ , the upper spectral bound in (4.3) reads  $\Theta_\alpha = \max\{\psi_2(\eta) : \psi_{p+2}(\eta) = 0\}$ . The assertion follows from Theorem 20 and the interlacing property of the zeros of real orthogonal polynomials (cf. [11, Theorem 1.20]).  $\square$

Can we proceed in the same way in order to compute the eigenvalues of the next matrix in turn, i.e., the stochastic Galerkin matrix  $U_{3,p}$ ? Following the lines of proof of Lemma 19, it is easy to establish a seven-term recurrence relation for the product  $\psi_3\psi_k$ . In fact, as we will see in the proof of Lemma 23, the product  $\psi_n\psi_k$  of any two orthonormal polynomials generated by an even weight function can be expressed in terms of the polynomials  $\psi_\ell$ , with degree  $\ell$  satisfying the relation  $|n-k| \leq \ell \leq n+k$  and  $n+k+\ell$  is an even integer. Thus, the product  $\psi_n\psi_k$  satisfies a  $(2n+1)$ -term recurrence relation.

LEMMA 22. For even weight functions the polynomial sequence  $\{\psi_3\psi_k\}_{k \geq 0}$  satisfies the seven-term recurrence relation

$$\begin{aligned} \psi_3(\xi)\psi_k(\xi) &= c_3\sqrt{\beta_{k+3}\beta_{k+2}\beta_{k+1}}\psi_{k+3}(\xi) + c_3\sqrt{\beta_k\beta_{k-1}\beta_{k-2}}\psi_{k-3}(\xi) \\ &\quad + (c_3(\beta_{k+2} + \beta_{k+1} + \beta_k) + c_1)\psi_{k+1}(\xi) \\ &\quad + (c_3(\beta_{k+1} + \beta_k + \beta_{k-1}) + c_1)\psi_{k-1}(\xi), \quad k = 0, 1, 2, \dots, \end{aligned} \tag{4.16}$$

where  $\psi_3(\xi) = c_3\xi^3 + c_1\xi$ , and  $\psi_k(\xi) \equiv 0$  for  $k = -1, -2, -3$ .

We omit the technical proof and utilize the recurrence relation (4.16) in the by now well established way:

$$\psi_3(\xi) \begin{bmatrix} \psi_0(\xi) \\ \psi_1(\xi) \\ \vdots \\ \psi_{p-2}(\xi) \\ \psi_{p-1}(\xi) \\ \psi_p(\xi) \end{bmatrix} = U_{3,p} \begin{bmatrix} \psi_0(\xi) \\ \psi_1(\xi) \\ \vdots \\ \psi_{p-2}(\xi) \\ \psi_{p-1}(\xi) \\ \psi_p(\xi) \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ c_3\sqrt{\beta_{p+1}\beta_p\beta_{p-1}}\psi_{p+1}(\xi) \\ c_3\sqrt{\beta_{p+2}\beta_{p+1}\beta_p}\psi_{p+2}(\xi) \\ c_3\sqrt{\beta_{p+3}\beta_{p+2}\beta_{p+1}}\psi_{p+3}(\xi) + r(\xi) \end{bmatrix}, \tag{4.17}$$

where  $r(\xi) = (c_3(\beta_{p+2} + \beta_{p+1} + \beta_p) + c_1)\psi_{p+1}(\xi)$ . To answer the question above, it is not obvious in which way, if at all, one could use the matrix equation (4.17) for the eigenvalue computation of  $U_{3,p}$ . The idea of reordering, which was applied successfully for the eigenvalue computation of  $U_{2,p}$ ,

does not lead to a decoupling of the matrix  $U_{3,p}$ , resulting instead in a block antidiagonal matrix. Moreover, when using (4.17), we assume the eigenvectors of  $U_{3,p}$  to have a special structure, an approach which might be misleading.

**5. Sparsity of Stochastic Galerkin matrices.** In this section we investigate the sparsity pattern of the Stochastic Galerkin matrices  $\mathbf{G}_\alpha$  in (2.6), where we assume even probability density functions  $\rho_m$ , see (4.6). In particular, we derive upper bounds on the number of nonzero entries of the univariate Stochastic Galerkin matrices  $U_n$  in (2.10), and of the matrices  $\mathbf{G}_\alpha$  where  $|\alpha| = 1$  for the space of complete polynomials  $\mathcal{V} = \mathcal{V}_p^C$ . Information on the sparsity pattern is useful for the efficient implementation of matrix-vector-multiplication with Stochastic Galerkin matrices.

**5.1. The univariate case.** We first specialize the linearization formula (2.15) for even weight functions. Again we omit the sub- and superscripts  $m$  which distinguish the random variables and weight functions.

LEMMA 23. *The product of any two orthonormal polynomials  $\psi_i$  and  $\psi_j$  associated with an even weight function has the representation*

$$\psi_i(\xi)\psi_j(\xi) = \sum_{\substack{k=|i-j|, \\ i+j+k \text{ is even}}}^{i+j} g_{kij} \psi_k(\xi). \quad (5.1)$$

*Proof.* Following an idea given by Market [18, Section 1] we deduce a recurrence relation for the product  $\psi_i\psi_j$  utilizing the reordered three-term recurrence relation in (4.9):

$$\begin{aligned} 0 &= \xi\psi_i(\xi)\psi_j(\xi) - \xi\psi_j(\xi)\psi_i(\xi) \\ &= \sqrt{\beta_i}\psi_{i-1}(\xi)\psi_j(\xi) + \sqrt{\beta_{i+1}}\psi_{i+1}(\xi)\psi_j(\xi) - \sqrt{\beta_j}\psi_{j-1}(\xi)\psi_i(\xi) - \sqrt{\beta_{j+1}}\psi_{j+1}(\xi)\psi_i(\xi), \end{aligned}$$

hence

$$\psi_i\psi_j = \frac{\sqrt{\beta_i}}{\sqrt{\beta_j}}\psi_{i-1}\psi_{j-1} + \frac{\sqrt{\beta_{i+1}}}{\sqrt{\beta_j}}\psi_{i+1}\psi_{j-1} - \frac{\sqrt{\beta_{j-1}}}{\sqrt{\beta_j}}\psi_i\psi_{j-2}. \quad (5.2)$$

For  $j = 1, \dots, i$  the product  $\psi_i\psi_j$  can be traced back to the initial products  $\psi_k\psi_0 = \psi_k$ ,  $k = i - j, i - j + 2, \dots, i + j - 2, i + j$ , cf. Figure 5.1. In addition the polynomials  $\psi_k$  on the right-hand side of (5.1) must have the same parity as the product  $\psi_i\psi_j$ , hence  $i + j + k$  is even in all cases.  $\square$

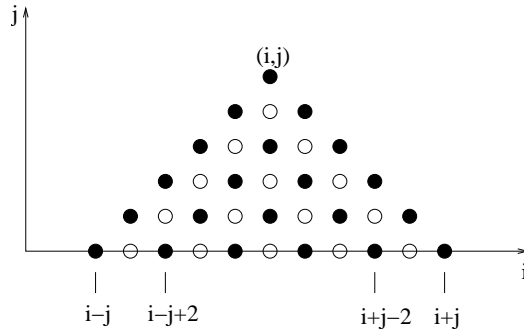


FIG. 5.1. Visualization of recurrence relation (5.2).

We note that by orthonormality we have  $g_{kij} = \langle \psi_k \psi_i \psi_j \rangle = [U_k]_{i,j}$  in (5.1), cf. Section 2.4. Thus, for even weight functions we obtain the following necessary condition for vanishing entries of  $U_n$ :

COROLLARY 24. For even weight functions,  $[U_n]_{i,j} \neq 0$  implies  $|i-j| \leq n \leq i+j$  and  $i+j+n$  is even.

The number of nonzero entries of  $U_n$  may be bounded as follows.

LEMMA 25.

(a) In case  $n = 2k$ ,  $k \in \mathbb{N}_0$ ,

$$\text{nnz}(U_n) \leq \begin{cases} (p-n+1)(n+1) + k^2, & 0 \leq n \leq p, \\ (p-k+1)^2, & p+1 \leq n \leq 2p, \\ 0, & n > 2p. \end{cases}$$

(b) In case  $n = 2k+1$ ,  $k \in \mathbb{N}_0$ ,

$$\text{nnz}(U_n) \leq \begin{cases} (p-n+1)(n+1) + k^2 + k, & 0 \leq n \leq p, \\ (p-k+1)(p-k), & p+1 \leq n \leq 2p, \\ 0, & n > 2p. \end{cases}$$

*Proof.*

We distinguish three cases:

- (1)  $n > 2p$ : by Proposition 4 we have  $U_n = O$ , i.e.,  $\text{nnz}(U_n) = 0$ .
- (2)  $p+1 \leq n \leq 2p$ :  $0 \leq i, j \leq p$  implies  $|i-j| \leq p$ , hence the necessary condition in Corollary 24 reduces to  $n \leq i+j$  and  $i+j+n$  is even. Note that matrix positions with  $i+j = n$  are admissible since  $i+j+n = n+n = 2n$  is always even. We count the number of admissible matrix positions running along the anti-diagonals of the matrix.

- If  $n = 2k$ ,  $k \in \mathbb{N}$ , is even, so is  $i+j$  meaning that entries on the main diagonal of  $U_n$  are admissible, see Figure 5.3(a):

$$\text{nnz}(U_n) \leq \sum_{s=0}^{p-k} 2s+1 = (p-k+1) + (p-k)(p-k+1) = (p-k+1)^2$$

- If  $n = 2k+1$ ,  $k \in \mathbb{N}_0$ , is odd, so is  $i+j$  meaning that entries on the main diagonal of  $U_n$  are not admissible, see Figure 5.3(b):

$$\text{nnz}(U_n) \leq \sum_{s=1}^{p-k} 2s = (p-k)(p-k+1)$$

- (3)  $0 \leq n \leq p$ : As in case (2) matrix positions with  $i+j = n$  are admissible. In addition positions that satisfy  $|i-j| = n$  are admissible since  $i+j+n = j \pm n + j + n = 2j + n \pm n$  is always even. Again we count the number of admissible matrix positions running along the anti-diagonals of the matrix  $U_n$ .

- If  $n = 2k$ ,  $k \in \mathbb{N}_0$ , is even, entries on the main diagonal of  $U_n$  are admissible, see Figure 5.2(a):

$$\begin{aligned} \text{nnz}(U_n) &\leq (p+1-n)(n+1) + \sum_{s=0}^{k-1} 2s+1 = (p+1-n)(n+1) + k + (k-1)k \\ &= (p+1-n)(n+1) + k^2 \end{aligned}$$

- If  $n = 2k+1$ ,  $k \in \mathbb{N}_0$ , is odd, entries on the main diagonal of  $U_n$  are not admissible, see Figure 5.2(b):

$$\text{nnz}(U_n) \leq (p+1-n)(n+1) + \sum_{s=1}^k 2s = (p+1-n)(n+1) + k^2 + k$$

□

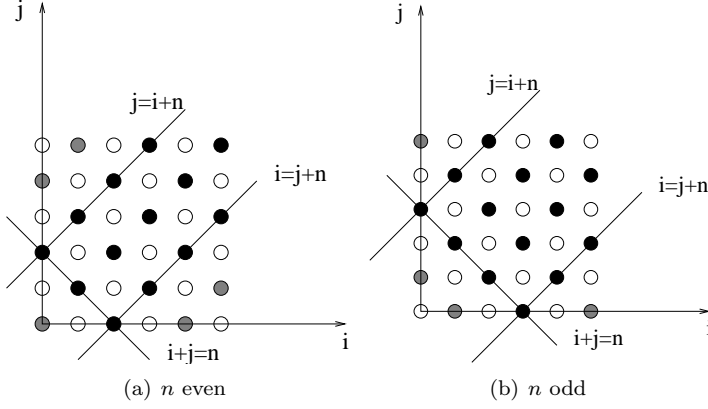


FIG. 5.2. Nonzero entries of  $U_n$  for  $0 \leq n \leq p$ .

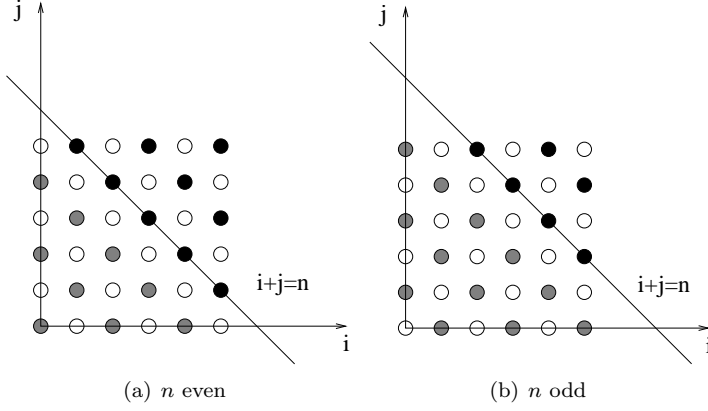


FIG. 5.3. Nonzero entries of  $U_n$  for  $p+1 \leq n \leq 2p$ .

The bounds given in Lemma 25 are sharp, since we count the exact number of nonzero entries provided that every admissible entry in  $U_n$  is not zero. This is true, for example, for the standard Gaussian probability density function, cf. (A.1) in the appendix and Figure 5.4.

**5.2. The multivariate case.** Since the entries of a stochastic Galerkin matrix (2.6) decouple into products of the form  $\langle \psi_{\alpha_m}^{(m)} \psi_{\beta_m}^{(m)} \psi_{\gamma_m}^{(m)} \rangle =: g_{\alpha_m \beta_m \gamma_m}^{(m)}$  for all  $m = 1, \dots, M$ , utilizing (5.1) we arrive at

PROPOSITION 26. For even weight functions,  $\alpha \in \mathcal{I}_a$  and  $\beta, \gamma \in \mathcal{I}$ , where  $\mathcal{I} = \mathcal{I}_p$  and  $\mathcal{I}_a = \mathcal{I}_{2p}$  or  $\mathcal{I} = \mathcal{I}_p^C$  and  $\mathcal{I}_a = \mathcal{I}_{2p}^C$ , respectively, the entries of the Stochastic Galerkin matrices in (2.6) read

$$[\mathbf{G}_\alpha]_{\beta, \gamma} = \langle \psi_\alpha \psi_\beta \psi_\gamma \rangle = \begin{cases} \prod_{m=1}^M g_{\alpha_m \beta_m \gamma_m}^{(m)}, & |\beta_m - \gamma_m| \leq \alpha_m \leq \beta_m + \gamma_m \\ & \text{and } \alpha_m + \beta_m + \gamma_m \text{ is even,} \\ 0, & \text{otherwise.} \end{cases}$$

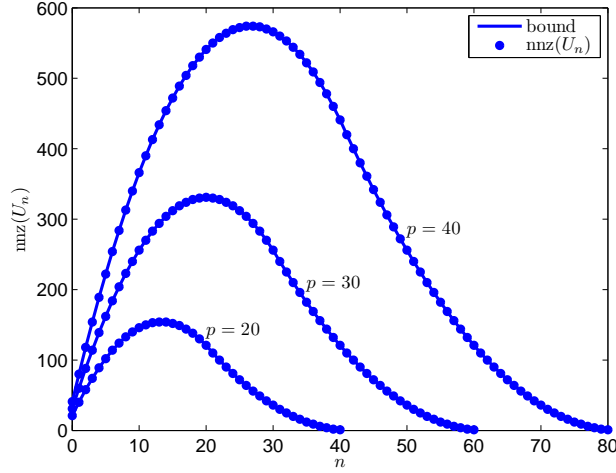


FIG. 5.4. Number of nonzero entries of  $U_n$  for a standard Gaussian probability density function and  $p = 20, 30, 40$ .

As a consequence, for the determination of the sparsity structure of each individual matrix  $\mathbf{G}_\alpha$ , we look for a description of all pairs of multi-indices in the set

$$N_\alpha = \{(\boldsymbol{\beta}, \boldsymbol{\gamma}) \in \mathcal{I} \times \mathcal{I} : |\beta_m - \gamma_m| \leq \alpha_m \leq \beta_m + \gamma_m, \alpha_m + \beta_m + \gamma_m \text{ is even}, m = 1, \dots, M\}, \quad (5.3)$$

where  $\mathcal{I}$  denotes either  $\mathcal{I}_p$  or  $\mathcal{I}_p^C$ , because only these multi-indices are associated with nonzero entries in  $\mathbf{G}_\alpha$ . Counting all admissible pairs of multi-indices will provide us at least an upper bound for the number of nonzero entries in  $\mathbf{G}_\alpha$ .

LEMMA 27. For the space of tensor product polynomials  $\mathcal{V} = \mathcal{V}_p$  there holds

$$\text{nnz}(\mathbf{G}_\alpha) \leq \prod_{m=1}^M \text{nnz}(U_{\alpha_m}^{(m)}). \quad (5.4)$$

*Proof.* This assertion follows from (2.11) and properties of the Kronecker product.  $\square$

We note that the bound in (5.4) holds for all weight functions regardless of their symmetry properties. For even weight functions, however, we have derived upper bounds for the univariate factors  $\text{nnz}(U_{\alpha_m}^{(m)})$  in (5.4) in the proof of Lemma 25. In addition, since these bounds are sharp, the bound given in Lemma 27 is also sharp for this special case.

LEMMA 28. For the space of complete polynomials  $\mathcal{V} = \mathcal{V}_p^C$  and  $|\alpha| = 1$  there holds, assuming even weight functions,

$$\text{nnz}(\mathbf{G}_\alpha^C) \leq 2 \binom{M+p-1}{p-1}.$$

*Proof.* Let  $\alpha_m = 1$  and  $\alpha_k = 0$  for  $m \neq k$ . It is easy to see that the set of admissible pairs of multi-indices given in (5.3) simplifies to

$$N_\alpha = \{(\boldsymbol{\beta}, \boldsymbol{\gamma}) \in \mathcal{I}_p^C \times \mathcal{I}_p^C : \beta_k = \gamma_k, k \neq m, |\beta_m - \gamma_m| = 1\}.$$



TABLE A.1

Orthonormal basis polynomials associated with common weight functions. The last column refers to the entries of the corresponding Stochastic Galerkin matrices  $U_n$  provided in the appendix.

Polynomial	Weight: $\rho(\xi)$	Support: $\Gamma$	Basis: $\psi_k(\xi)$	$[U_n]_{i,j}$
$H_k(\xi)$ : Hermite	$\frac{1}{\sqrt{2\pi}}e^{-\xi^2/2}$	$\mathbb{R}$	$\frac{1}{\sqrt{2^k k!}}H_k\left(\frac{\xi}{\sqrt{2}}\right)$	(A.1)
$P_k(\xi)$ : Legendre	$\frac{1}{2\sqrt{3}}$	$]-\sqrt{3}, \sqrt{3}[$	$\sqrt{2k+1}P_k\left(\frac{\xi}{\sqrt{3}}\right)$	(A.2)
$T_k(\xi)$ : Chebyshev (first kind)	$\frac{1}{\pi}\frac{1}{\sqrt{2-\xi^2}}$	$]-\sqrt{2}, \sqrt{2}[$	$\sqrt{2-\delta_{0,k}}T_k\left(\frac{\xi}{\sqrt{2}}\right)$	(A.3)
$U_k(\xi)$ : Chebyshev (second kind)	$\frac{1}{2\pi}\sqrt{4-\xi^2}$	$]-2, 2[$	$U_k\left(\frac{\xi}{2}\right)$	(A.4)

In addition the multi-indices  $\beta, \gamma \in \mathcal{I}_p^C$  must satisfy  $|\beta| \leq p$  and  $|\gamma| \leq p$ . Consider the case  $\beta_m = \gamma_m + 1$ . We obtain all admissible pairs  $(\beta, \gamma)$  in the following way: First fix  $\beta_m = 1$  and  $\gamma_m = 0$ . The remaining  $M - 1$  positions can be filled with all configurations such that their sum is less than or equal to  $p - 1$ , meaning that we list all polynomials in  $M - 1$  variables of total degree not larger than  $p - 1$ . Next we choose  $\beta_m = 2$ ,  $\gamma_m = 1$  and list all polynomials in  $M - 1$  variables of total degree not larger than  $p - 2$  and so on up to  $\beta_m = p$  and  $\gamma_m = p - 1$ . Thus the number of admissible pairs is

$$\sum_{\ell=1}^p \binom{M-1+p-\ell}{p-\ell} = \sum_{n=0}^{p-1} \binom{M-1+n}{n} = \binom{M-1+p-1+1}{p-1} = \binom{M+p-1}{M}.$$

The second case  $\gamma_m = \beta_m + 1$  generates the same number of admissible pairs by simply interchanging the role of  $\beta_m$  and  $\gamma_m$ , hence  $\text{nnz}(\mathbf{G}_\alpha^C) \leq 2 \binom{M+p-1}{M}$ .  $\square$

We note that sparsity results for the stochastically nonlinear case could also be investigated for the individual matrices  $\{\mathbf{G}_\alpha\}_{\alpha \in \mathcal{I}_a}$ . However, in this case the full Galerkin matrix (2.5) consisting of a linear combination of these matrices is essentially fully populated in the sense that, for each pair of multi-indices  $(\beta, \gamma) \in \mathcal{I} \times \mathcal{I}$  there is a multi-index  $\alpha \in \mathcal{I}_a$  such that  $[\mathbf{G}_\alpha]_{\beta, \gamma} \neq 0$ . There is, therefore, little sparsity to exploit.

**6. Conclusions.** We have presented a discussion of the structure as well as spectral and sparsity properties of the matrices occurring in the Stochastic Galerkin discretization of linear PDEs with random coefficients. Besides being helpful in the implementation of Stochastic Galerkin schemes, such results are crucial for the design and analysis of efficient iterative solution methods. In particular, if the coefficient function depends linearly on a finite number of independent random variables, we have shown that employing the space of complete polynomials for the discretization of the stochastic function space precludes the decoupling of the stochastic degrees of freedom. By consequence, it is then necessary to solve a large fully coupled linear system of Galerkin equations involving all stochastic and deterministic degrees of freedom. Finally, Stochastic Galerkin matrices possess interesting structural properties and provide challenging matrix eigenvalue problems, for which we have given a partial solution.

### Appendix A. Linearization coefficients.

We collect the nonzero entries of the Stochastic Galerkin matrices  $U_n$  defined in (2.10) for systems of orthonormal basis polynomials associated with common weight functions. In Section 2.4 we have identified the matrix entry  $[U_n]_{i,j}$  as linearization coefficient  $g_{nij}$ , cf. (2.15). The basis polynomials  $\{\psi_k\}_{k \in \mathbb{N}_0}$  along with their corresponding weight function  $\rho$  and support  $\Gamma$  are defined in Table A.1.

**A.1. Standard Gaussian distribution.** The linearization coefficients for the Hermite polynomials  $\{H_k\}_{k \in \mathbb{N}_0}$  are given e.g. in [9, Chapter XVI, Section 16.5] and [4, Lecture 5]. Normalization as defined in Table A.1 yields the entries of the Stochastic Galerkin matrices  $U_n$  corresponding to the standard Gaussian weight function:

$$[U_n]_{i,j} = \begin{cases} \frac{\sqrt{i!j!n!}}{s!(i-s)!(j-s)!}, & s = \frac{i+j-n}{2}, \quad i+j-n \text{ even}, |i-j| \leq n \leq i+j, \\ 0, & \text{otherwise.} \end{cases} \quad (\text{A.1})$$

**A.2. Uniform distribution.** We utilize the linearization coefficients for the Legendre polynomials  $\{P_k\}_{k \in \mathbb{N}_0}$  given in [1]. Normalizing the Legendre polynomials as defined in Table A.1 we arrive at

$$[U_n]_{i,j} = \begin{cases} \frac{\sqrt{(2i+1)(2j+1)(2n+1)}}{i+j+n+1} \frac{A(s-i)A(s-j)A(s-n)}{A(s)}, & s = \frac{i+j+n}{2}, \quad i+j+n \text{ even}, \\ & |i-j| \leq n \leq i+j, \\ 0, & \text{otherwise,} \end{cases} \quad (\text{A.2})$$

for the uniform weight function. Above, we have introduced the function

$$A(n) = \begin{cases} \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{n!}, & n \geq 1, \\ 1, & n = 0, \\ 0, & n < 0. \end{cases}$$

**A.3. Beta(1/2,1/2) distribution.** The product of any two Chebyshev polynomials of first kind can be expressed as

$$T_i(\xi)T_j(\xi) = (T_{i+j}(\xi) + T_{|i-j|}(\xi)) / 2,$$

see for example [3, Section 5.1]. Hence the linearization coefficients for the Chebyshev polynomials of first kind are given by  $\langle T_i T_j T_n \rangle = \frac{1}{2} (\delta_{i+j,n} + \delta_{|i-j|,n})$ ,  $i, j, n \geq 0$ . Normalization of the Chebyshev polynomials (see Table A.1) yields

$$[U_n]_{i,j} = \begin{cases} 1, & n = 0, i = j \geq 0, \\ 1, & i = 0, j = n > 0, \\ 1, & j = 0, i = n > 0, \\ \frac{1}{\sqrt{2}} (\delta_{i+j,n} + \delta_{|i-j|,n}), & i, j, n > 0, i+j-n \text{ even}, |i-j| \leq n \leq i+j, \\ 0, & \text{otherwise,} \end{cases} \quad (\text{A.3})$$

for the Beta(1/2,1/2) probability density function.

**A.4. Beta(3/2,3/2) distribution.** The product of any two Chebyshev polynomials of second kind can be expressed as

$$U_i(\xi)U_j(\xi) = \sum_{\ell=0}^{\min(i,j)} U_{i+j-2\ell}(\xi),$$

see for example [3, Section 5.1]. Thus the linearization coefficients for the Chebyshev polynomials of second kind are one for  $i+j-n$  even and  $|i-j| \leq n \leq i+j$  and are zero otherwise. Utilizing the definition in Table A.1 we obtain

$$[U_n]_{i,j} = \begin{cases} 1, & i+j-n \text{ even}, |i-j| \leq n \leq i+j, \\ 0, & \text{otherwise,} \end{cases} \quad (\text{A.4})$$

for the Beta(1/2,1/2) probability density function.

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