## SPECTRAL METHODS FOR PARAMETERIZED MATRIX EQUATIONS

PAUL G. CONSTANTINE\*, DAVID F. GLEICH<sup>†</sup>, AND GIANLUCA IACCARINO<sup>‡</sup>

**Abstract.** We apply polynomial approximation methods — known in the numerical PDEs context as *spectral methods* — to approximate the vector-valued function that satisfies a linear system of equations where the matrix and the right hand side depend on a parameter. We derive both an interpolatory pseudospectral method and a residual-minimizing Galerkin method, and we show how each can be interpreted as solving a truncated infinite system of equations; the difference between the two methods lies in where the truncation occurs. Using classical theory, we derive asymptotic error estimates related to the region of analyticity of the solution, and we present a practical residual error estimate. We verify the results with two numerical examples.

Key words. parameterized systems, spectral methods

1. Introduction. We consider a system of linear equations where the elements of the matrix of coefficients and right hand side depend analytically on a parameter. Such systems often arise as an intermediate step within computational methods for engineering models which depend on one or more parameters. A large class of models employ such parameters to represent uncertainty in the input quantities; examples include PDEs with random inputs [2, 13, 29], image deblurring models [8], and noisy inverse problems [7]. Other examples of parameterized linear systems occur in electronic circuit design [22], applications of PageRank [5, 9], and dynamical systems [10]. Additionally, we note a recent rational interpolation scheme proposed by Wang et al. [27] where each evaluation of the interpolant involves a constrained least-squares problem that depends on the point of evaluation. Parameterized linear operators have been analyzed in their own right in the context of perturbation theory; the standard reference for this work is Kato [21].

In our case, we are interested in approximating the vector-valued function that satisfies the parameterized matrix equation. We will analyze the use of polynomial approximation methods, which have evolved under the heading "spectral methods" in the context of numerical methods for PDEs [3, 6, 20]. In their most basic form, these methods are characterized by a global approximation of the function of interest by a finite series of orthogonal (algebraic or trigonometric) polynomials. For smooth functions, these methods converge geometrically, which is the primary reason for their popularity. The use of spectral methods for parameterized equations is not unprecedented. In fact, the authors were motivated primarily by the so-called polynomial chaos methods [16, 29] and related work [2, 1, 28] in the burgeoning field of uncertainty quantification. There has been some work in the linear algebra community analyzing the fully discrete problems that arise in this context [12, 24, 11], but we know of no existing work addressing the more general problem of parameterized matrix equations.

There is an ongoing debate in spectral methods communities surrounding the relative advantages of Galerkin methods versus pseudospectral methods. In the case of pa-

<sup>\*</sup>Institute for Computational and Mathematical Engineering, Stanford University, Stanford, California, 94305 (paul.constantine@stanford.edu).

<sup>&</sup>lt;sup>†</sup>Institute for Computational and Mathematical Engineering, Stanford University, Stanford, California, 94305 (dgleich@stanford.edu).

<sup>&</sup>lt;sup>‡</sup>Institute for Computational and Mathematical Engineering, Department of Mechanical Engineering, Stanford University, Stanford, California, 94305 (jops@stanford.edu).

TABLE	1		1
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We attempt to use a consistent and clear notation throughout the paper. This table details the notational conventions, which we use unless otherwise noted. Also, all indices begin at 0.

Notation	Meaning
A(s)	a square matrix-valued function of a parameter $s$
b(s)	a vector-valued function of the parameter $s$
$\mathbf{A}$	a constant matrix
b	a constant vector
$\langle \cdot \rangle$	the integral with respect to a given weight function
$\langle \cdot \rangle_n$	the integral $\langle \cdot \rangle$ approximated by an <i>n</i> -point Gauss quadrature rule
$\left[\mathbf{M} ight]_{r imes r}$	the first $r \times r$ principal minor of a matrix <b>M</b>

rameterized matrix equations, the interpolatory pseudospectral methods only require the solution of the parameterized model evaluated at a discrete set of points, which makes parallel implementation straightforward. In contrast, the Galerkin method requires the solution of a coupled linear system whose dimension is many times larger than the original parameterized set of equations. We offer insight into this contest by establishing a fair ground for rigorous comparison and deriving a concrete relationship between the two methods.

In this paper, we will first describe the parameterized matrix equation and characterize its solution in section 2. We then derive a spectral Galerkin method and a pseudospectral method for approximating the solution to the parameterized matrix equation in section 3. In section 4, we analyze the relationship between these methods using the symmetric, tridiagonal Jacobi matrices – techniques which are reminiscent of the analysis of Gauss quadrature by Golub and Meurant [17] and Gautschi [14]. We derive error estimates for the methods that relate the geometric rate of convergence to the size of the region of analyticity of the solution in section 5, and we conclude with simple numerical examples in section 6. See table 1 for a list of notational conventions, and note that all index sets begin at 0 to remain consistent with the ordering of a set of polynomials by their largest degree.

2. Parameterized Matrix Equations. In this section, we define the specific problem we will study and characterize its solution. We consider problems that depend on a single parameter s that takes values in the finite interval [-1,1]. Assume that the interval [-1,1] is equipped with a positive scalar weight function w(s) such that all moments exist, i.e.

$$\langle s^k \rangle \equiv \int_{-1}^1 s^k w(s) \, ds < \infty, \qquad k = 1, 2, \dots,$$
 (2.1)

and the integral of w(s) is equal to 1. We will use the bracket notation to denote an integral against the given weight function. In a stochastic context, one may interpret this as an expectation operator where w(s) is the density function of the random variable s.

Let the  $\mathbb{R}^N$ -valued function x(s) satisfy the linear system of equations

$$A(s)x(s) = b(s), \qquad s \in [-1, 1]$$
 (2.2)

for a given  $\mathbb{R}^{N \times N}$ -valued function A(s) and  $\mathbb{R}^{N}$ -valued function b(s). We assume that both A(s) and b(s) are analytic in a region containing [-1, 1], which implies that they

have a convergent power series

$$A(s) = \mathbf{A}_0 + \mathbf{A}_1 s + \mathbf{A}_2 s^2 + \cdots, \qquad b(s) = \mathbf{b}_0 + \mathbf{b}_1 s + \mathbf{b}_2 s^2 + \cdots, \qquad (2.3)$$

for some constant matrices  $\mathbf{A}_i$  and constant vectors  $\mathbf{b}_i$ . Additionally, we assume that A(s) is bounded away from singularity for all  $s \in [-1, 1]$ . This implies that we can write  $x(s) = A^{-1}(s)b(s)$ .

The elements of the solution x(s) can also be written using Cramer's rule [23, Chapter 6] as a ratio of determinants.

$$x_i(s) = \frac{\det(A_i(s))}{\det(A(s))}, \qquad i = 0, \dots, N-1,$$
 (2.4)

where  $A_i(s)$  is the parameterized matrix formed by replacing the *i*th column of A(s) by b(s). From equation (2.4) and the invertibility of A(s), we can conclude that x(s) is analytic in a region containing [-1, 1].

Equation (2.4) reveals the underlying structure of the solution as a function of s. If A(s) and b(s) depend polynomially on s, then (2.4) tells us that x(s) is a rational function. Note also that this structure is independent of the particular weight function w(s).

3. Spectral Methods. In this section, we derive the spectral methods we use to approximate the solution x(s). We begin with a brief review of the relevant theory of orthogonal polynomials, Gaussian quadrature, and Fourier series. We include this section primarily for the sake of notation and refer the reader to a standard text on orthogonal polynomials [26] for further theoretical details and [15] for a modern perspective on computation.

**3.1. Orthogonal Polynomials and Gaussian Quadrature.** Let  $\mathbb{P}$  be the space of real polynomials defined on [-1, 1], and let  $\mathbb{P}_n \subset \mathbb{P}$  be the space of polynomials of degree at most n. For any p, q in  $\mathbb{P}$ , we define the inner product as

$$\langle pq \rangle \equiv \int_{-1}^{1} p(s)q(s)w(s) \, ds. \tag{3.1}$$

We define a norm on  $\mathbb{P}$  as  $\|p\|_{L^2} = \sqrt{\langle p^2 \rangle}$ , which is the standard  $L^2$  norm for the given weight w(s). Let  $\{\pi_k(s)\}$  be the set of polynomials that are orthonormal with respect to w(s), i.e.  $\langle \pi_i \pi_j \rangle = \delta_{ij}$ . It is known that  $\{\pi_k(s)\}$  satisfy the three-term recurrence relation

$$\beta_{k+1}\pi_{k+1}(s) = (s - \alpha_k)\pi_k(s) - \beta_k\pi_{k-1}(s), \qquad k = 0, 1, 2, \dots,$$
(3.2)

with  $\pi_{-1}(s) = 0$  and  $\pi_0(s) = 1$ . If we consider only the first *n* equations, then we can rewrite (3.2) as

$$s\pi_k(s) = \beta_k \pi_{k-1}(s) + \alpha_k \pi_k(s) + \beta_{k+1} \pi_{k+1}(s), \qquad k = 0, 1, \dots, n-1.$$
(3.3)

Setting  $\boldsymbol{\pi}_n(s) = [\pi_0(s), \pi_1(s), \dots, \pi_{n-1}(s)]^T$ , we can write this conveniently in matrix form as

$$s\boldsymbol{\pi}_n(s) = \mathbf{J}_n \boldsymbol{\pi}_n(s) + \beta_n \boldsymbol{\pi}_n(s) \mathbf{e}_n \tag{3.4}$$

where  $\mathbf{e}_n$  is a vector of zeros with a one in the last entry, and  $\mathbf{J}_n$  (known as the *Jacobi* matrix) is a symmetric, tridiagonal matrix defined as

$$\mathbf{J}_{n} = \begin{bmatrix} \alpha_{0} & \beta_{1} & & & \\ \beta_{1} & \alpha_{1} & \beta_{2} & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n-2} & \alpha_{n-2} & \beta_{n-1} \\ & & & & \beta_{n-1} & \alpha_{n-1} \end{bmatrix}.$$
 (3.5)

The zeros  $\{\lambda_i\}$  of  $\pi_n(s)$  are the eigenvalues of  $\mathbf{J}_n$  and  $\pi_n(\lambda_i)$  are the corresponding eigenvectors; this follows directly from (3.4). Let  $\mathbf{Q}_n$  be the orthogonal matrix of eigenvectors of  $\mathbf{J}_n$ . Then we write the eigenvalue decomposition of  $\mathbf{J}_n$  as

$$\mathbf{J}_n = \mathbf{Q}_n \mathbf{\Lambda}_n \mathbf{Q}_n^T. \tag{3.6}$$

It is known (c.f. [15]) that the eigenvalues  $\{\lambda_i\}$  are the familiar Gaussian quadrature points associated with the weight function w(s). The quadrature weight  $\nu_i$  corresponding to  $\lambda_i$  is equal to the square of the first component of the eigenvector associated with  $\lambda_i$ , i.e.

$$\mathbf{Q}(0,i)^2 = \nu_i. \tag{3.7}$$

The weights  $\{\nu_i\}$  are known to be strictly positive. We will use these facts repeatedly in the sequel. For an integrable scalar function f(s), we can approximate its integral by an *n*-point Gaussian quadrature rule, which is a weighted sum of function evaluations,

$$\int_{-1}^{1} f(s)w(s) \, ds = \sum_{i=0}^{n-1} f(\lambda_i)\nu_i + R_n(f). \tag{3.8}$$

If  $f \in \mathbb{P}_{2n-1}$ , then  $R_n(f) = 0$ ; that is to say the *degree of exactness* of the Gaussian quadrature rule is 2n - 1. We use the notation

$$\langle f \rangle_n \equiv \sum_{i=0}^{n-1} f(\lambda_i) \nu_i$$
 (3.9)

to denote the Gaussian quadrature rule. This is a discrete approximation to the true integral.

**3.2. Fourier Series.** The polynomials  $\{\pi_k(s)\}$  form an orthonormal basis for the Hilbert space

$$L^{2} \equiv L^{2}_{w}([-1,1]) = \{f : [-1,1] \to \mathbb{R} \mid \|f\|_{L^{2}} < \infty\}.$$
(3.10)

Therefore, any  $f \in L^2$  admits a convergent Fourier series

$$f(s) = \sum_{k=0}^{\infty} \langle f\pi_k \rangle \, \pi_k(s). \tag{3.11}$$

The coefficients  $\langle f\pi_k \rangle$  are called the *Fourier coefficients*. If we truncate the series (3.11) after n terms, we are left with a polynomial of degree n-1 that is the best approximation polynomial in the  $L^2$  norm. In other words, if we denote

$$P_n f(s) = \sum_{k=0}^{n-1} \langle f \pi_k \rangle \, \pi_k(s), \qquad (3.12)$$

then

$$\|f - P_n f\|_{L^2} = \inf_{p \in \mathbb{P}_{n-1}} \|f - p\|_{L^2}.$$
(3.13)

In fact, the error made by truncating the series is equal to the sum of squares of the neglected coefficients,

$$\|f - P_n f\|_{L^2}^2 = \sum_{k=n}^{\infty} \langle f \pi_k \rangle^2.$$
(3.14)

These properties of the Fourier series motivate the theory and practice of spectral methods.

We have shown that the each element of the solution x(s) of the parameterized matrix equation is analytic in a region containing the closed interval [-1, 1]. Therefore it is continuous and bounded on [-1, 1], which implies that  $x_i(s) \in L^2$  for  $i = 0, \ldots, N-1$ . We can thus write the convergent Fourier expansion for each element using vector notation as

$$x(s) = \sum_{k=0}^{\infty} \langle x\pi_k \rangle \, \pi_k(s). \tag{3.15}$$

Note that we are abusing the bracket notation here, but this will make further manipulations very convenient. The computational strategy is to choose a truncation level n-1 and estimate the coefficients of the truncated expansion.

**3.3. Spectral Collocation.** The term *spectral collocation* typically refers to the technique of constructing a Lagrange interpolating polynomial through the exact solution evaluated at the Gaussian quadrature points. Suppose that  $\lambda_i$ ,  $i = 0, \ldots, n-1$  are the Gaussian quadrature points for the weight function w(s). We can construct an n-1 degree polynomial interpolant of the solution through these points as

$$x_{c,n}(s) = \sum_{i=0}^{n-1} x(\lambda_i)\ell_i(s) \equiv \mathbf{X}_c \mathbf{l}_n(s).$$
(3.16)

The vector  $x(\lambda_i)$  is the solution to the equation  $A(\lambda_i)x(\lambda_i) = b(\lambda_i)$ . The n-1 degree polynomial  $\ell_i(s)$  is the standard Lagrange basis polynomial defined as

$$\ell_i(s) = \prod_{j=0, \ j\neq i}^{n-1} \frac{s - \lambda_j}{\lambda_i - \lambda_j}.$$
(3.17)

The  $N \times n$  constant matrix  $\mathbf{X}_c$  (the subscript *c* is for *collocation*) has one column for each  $x(\lambda_i)$ , and  $\mathbf{l}_n(s)$  is a vector of the Lagrange basis polynomials.

By construction, the collocation polynomial  $x_{c,n}$  interpolates the true solution x(s) at the Gaussian quadrature points. We will use this construction to show the connection between the pseudospectral method and the Galerkin method.

**3.4.** Pseudospectral Methods. Notice that computing the true coefficients of the Fourier expansion of x(s) requires the exact solution. The essential idea of the pseudospectral method is to approximate the Fourier coefficients of x(s) by a Gaussian quadrature rule. In other words,

$$x_{p,n}(s) = \sum_{i=0}^{n-1} \langle x\pi_k \rangle_n \pi_k(s) \equiv \mathbf{X}_p \boldsymbol{\pi}_n(s), \qquad (3.18)$$

where  $\mathbf{X}_p$  is an  $N \times n$  constant matrix of the approximated Fourier coefficients; the subscript p is for *pseudospectral*. For clarity, we recall

$$\langle x\pi_k \rangle_n = \sum_{i=0}^{n-1} x(\lambda_i)\pi_k(\lambda_i)\nu_i.$$
(3.19)

where  $x(\lambda_i)$  solves  $A(\lambda_i)x(\lambda_i) = b(\lambda_i)$ . In general, the number of points in the quadrature rule need not have any relationship to the order of truncation. However, when the number of terms in the truncated series is equal to the number of points in the quadrature rule, the pseudospectral approximation is equivalent to the collocation approximation. This relationship is well-known, but we include following lemma and theorem for use in later proofs.

LEMMA 3.1. Let  $\mathbf{q}_0$  be the first row of  $\mathbf{Q}_n$ , and define  $\mathbf{D}_{\mathbf{q}_0} = \text{diag}(\mathbf{q}_0)$ . The matrices  $\mathbf{X}_p$  and  $\mathbf{X}_c$  are related by the equation  $\mathbf{X}_p = \mathbf{X}_c \mathbf{D}_{\mathbf{q}_0} \mathbf{Q}_n^T$ .

$$\begin{aligned} \mathbf{X}_{p}(:,k) &= \langle x\pi_{k} \rangle_{n} \\ &= \sum_{j=0}^{n-1} x(\lambda_{j})\pi_{k}(\lambda_{j})\nu_{j} \\ &= \sum_{j=0}^{n-1} \mathbf{X}_{c}(:,j) \frac{1}{\|\boldsymbol{\pi}_{n}(\lambda_{j})\|_{2}} \frac{\pi_{k}(\lambda_{j})}{\|\boldsymbol{\pi}_{n}(\lambda_{j})\|_{2}} \\ &= \mathbf{X}_{c} \mathbf{D}_{\mathbf{q}_{0}} \mathbf{Q}_{n}^{T}(:,k) \end{aligned}$$

which implies  $\mathbf{X}_p = \mathbf{X}_c \mathbf{D}_{\mathbf{q}_0} \mathbf{Q}_n^T$  as required.  $\square$ 

THEOREM 3.2. The n-1 degree collocation approximation is equal to the n-1 degree pseudospectral approximation using an n-point Gaussian quadrature rule, i.e.

$$x_{c,n}(s) = x_{p,n}(s).$$
 (3.20)

for all s.

*Proof.* Note that the elements of  $\mathbf{q}_0$  are all non-zero, so  $\mathbf{D}_{\mathbf{q}_0}^{-1}$  exists. Then lemma 3.1 implies  $\mathbf{X}_c = \mathbf{X}_p \mathbf{Q}_n \mathbf{D}_{\mathbf{q}_0}^{-1}$ . Using this change of variables, we can write

$$x_{c,n}(s) = \mathbf{X}_c \mathbf{l}_n(s) = \mathbf{X}_p \mathbf{Q}_n \mathbf{D}_{\mathbf{q}_0}^{-1} \mathbf{l}_n(s).$$
(3.21)

Thus it is sufficient to show that  $\pi_n(s) = \mathbf{Q}_n \mathbf{D}_{\mathbf{q}_0}^{-1} \mathbf{l}_n(s)$ . Since this is just a vector of polynomials with degree at most n-1, we can do this by multiplying each element by each orthonormal basis polynomial up to order n-1 and integrating. Towards this end we define  $\mathbf{\Theta} \equiv \langle \mathbf{l}_n \pi_n^T \rangle$ .

Using the polynomial exactness of the Gaussian quadrature rule, we compute the i, j element of  $\Theta$ .

$$\Theta(i,j) = \langle l_i \pi_j \rangle$$
  
=  $\sum_{k=0}^{n-1} \ell_i(\lambda_k) \pi_j(\lambda_k) \nu_k$   
=  $\frac{1}{\|\pi_n(\lambda_i)\|_2} \frac{\pi_j(\lambda_i)}{\|\pi_n(\lambda_i)\|_2}$   
=  $\mathbf{Q}_n(0,i) \mathbf{Q}_n(j,i),$ 

which implies that  $\boldsymbol{\Theta} = \mathbf{D}_{\mathbf{q}_0} \mathbf{Q}_n^T$ . Therefore

$$egin{aligned} &\left\langle \mathbf{Q}_n \mathbf{D}_{\mathbf{q}_0}^{-1} \mathbf{l}_n \pi_n^T 
ight
angle &= \mathbf{Q}_n \mathbf{D}_{\mathbf{q}_0}^{-1} \left\langle \mathbf{l}_n \pi_n^T 
ight
angle \ &= \mathbf{Q}_n \mathbf{D}_{\mathbf{q}_0}^{-1} \mathbf{\Theta} \ &= \mathbf{Q}_n \mathbf{D}_{\mathbf{q}_0}^{-1} \mathbf{D}_{\mathbf{q}_0} \mathbf{Q}_n^T \ &= \mathbf{I}_n, \end{aligned}$$

which completes the proof.  $\square$ 

Some refer to the pseudospectral method explicitly as an interpolation method [3]. See [20] for an insightful interpretation in terms of a discrete projection. Because of this property, we will freely interchange the collocation and pseudospectral approximations when convenient in the ensuing analysis.

The work required to compute the pseudospectral approximation is highly dependent on the parameterized system. In general, we assume that the computation of  $x(\lambda_i)$  dominates the work; in other words, the cost of computing Gaussian quadrature formulas is negligible compared to computing the solution to each linear system. Then if each  $x(\lambda_i)$  costs  $\mathcal{O}(N^3)$ , the pseudospectral approximation with *n* terms costs  $\mathcal{O}(nN^3)$ .

**3.5.** Spectral Galerkin. The spectral Galerkin method computes a finite dimensional approximation to x(s) such that each element of the equation residual is orthogonal to the approximation space. Define

$$r(y,s) = A(s)y(s) - b(s).$$
(3.22)

The finite dimensional approximation space for each component  $x_i(s)$  will be the space of polynomials of degree at most n-1. This space is spanned by the first n orthonormal polynomials, i.e.  $\operatorname{span}(\pi_0(s), \ldots, \pi_{n-1}(s)) = \mathbb{P}_{n-1}$ . We seek an  $\mathbb{R}^N$ -valued polynomial  $x_{q,n}(s)$  of maximum degree n-1 such that

$$\langle r_i(x_{g,n})\pi_k \rangle = 0, \qquad i = 0, \dots, N-1, \qquad k = 0, \dots, n-1,$$
(3.23)

where  $r_i(x_{g,n})$  is the *i*th component of the residual. We can write equations (3.23) in matrix notation as

$$\left\langle r(x_{g,n})\boldsymbol{\pi}_{n}^{T}\right\rangle = \mathbf{0} \tag{3.24}$$

or equivalently

$$\langle Ax_{g,n}\boldsymbol{\pi}_n^T \rangle = \langle b\boldsymbol{\pi}_n^T \rangle.$$
 (3.25)

Since each component of  $x_{g,n}(s)$  is a polynomial of degree at most n-1, we can write its expansion in  $\{\pi_k(s)\}$  as

$$x_{g,n}(s) = \sum_{k=0}^{n-1} \mathbf{x}_{g,k} \pi_k(s) \equiv \mathbf{X}_g \pi_n(s),$$
 (3.26)

where  $\mathbf{X}_g$  is a constant matrix of size  $N \times n$ ; the subscript g is for *Galerkin*. Then equation (3.25) becomes

$$\langle A\mathbf{X}_g \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \rangle = \langle b \boldsymbol{\pi}_n^T \rangle.$$
 (3.27)

Using the vec notation [18, Section 4.5], we can rewrite (3.27) as

$$\langle \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \otimes A \rangle \operatorname{vec}(\mathbf{X}_g) = \langle \boldsymbol{\pi}_n \otimes b \rangle.$$
 (3.28)

where  $\operatorname{vec}(\mathbf{X}_g)$  is an  $Nn \times 1$  constant vector equal to the columns of  $\mathbf{X}_g$  stacked on top of each other. The constant matrix  $\langle \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \otimes A \rangle$  has size  $Nn \times Nn$  and a distinct block structure; the i, j block of size  $N \times N$  is equal to  $\langle \pi_i \pi_j A \rangle$ . More explicitly,

$$\left\langle \boldsymbol{\pi}_{n} \boldsymbol{\pi}_{n}^{T} \otimes A \right\rangle = \begin{bmatrix} \left\langle \pi_{0} \pi_{0} A \right\rangle & \cdots & \left\langle \pi_{0} \pi_{n-1} A \right\rangle \\ \vdots & \ddots & \vdots \\ \left\langle \pi_{n-1} \pi_{0} A \right\rangle & \cdots & \left\langle \pi_{n-1} \pi_{n-1} A \right\rangle \end{bmatrix}.$$
 (3.29)

Similarly, the *i*th block of the  $Nn \times 1$  vector  $\langle \pi_n \otimes b \rangle$  is equal to  $\langle b\pi_i \rangle$ , which is exactly the *i*th Fourier coefficient of b(s).

Since A(s) is bounded and nonsingular for all  $s \in [-1, 1]$ , it is straightforward to show that  $x_{g,n}(s)$  exists and is unique using the classical Galerkin theorems presented and summarized in Brenner and Scott [4, Chapter 2]. This implies that  $\mathbf{X}_g$  is unique, and since b(s) is arbitrary, we conclude that the matrix  $\langle \pi_n \pi_n^T \otimes A \rangle$  is nonsingular for all finite truncations n.

The work required to compute the Galerkin approximation depends on how one computes the integrals in equation (3.28). If we assume that the cost of forming the system is negligible, then the costly part of the computation is solving the system (3.28). The size of the matrix  $\langle \pi_n \pi_n^T \otimes A \rangle$  is  $Nn \times Nn$ , so we expect an operation count of  $\mathcal{O}(N^3 n^3)$ , in general. However, many applications beget systems with sparsity or exploitable structure that can considerably reduce the required work.

**3.6.** Summary. We have discussed two classes of spectral methods: (i) the interpolatory pseudospectral method which approximates the truncated Fourier series of x(s) by using a Gaussian quadrature rule to approximate each Fourier coefficient, and (ii) the Galerkin projection method which finds an approximation in a finite dimensional subspace such that the residual  $A(s)x_{g,n}(s) - b(s)$  is orthogonal to the approximation space. In general, the *n*-term pseudospectral approximation requires *n* solutions of the original parameterized matrix equation (2.2) evaluated at the Gaussian quadrature points, while the Galerkin method requires the solution of the coupled linear system of equations (3.28) that is *n* times as large as the original parameterized matrix equation. A rough operation count for the pseudospectral and Galerkin approximations is  $\mathcal{O}(nN^3)$  and  $\mathcal{O}(n^3N^3)$ , respectively.

Before discussing asymptotic error estimates, we first derive some interesting and useful connections between these two classes of methods. In particular, we can interpret each method as a set of functions acting on the infinite Jacobi matrix for the weight function w(s); the difference between the methods lies in where each truncates the infinite system of equations.

4. Connections Between Pseudospectral and Galerkin. We begin with a useful lemma for representing a matrix of Gauss quadrature integrals in terms of functions of the Jacobi matrix.

LEMMA 4.1. Let f(s) be a scalar function analytic in a region containing [-1,1]. Then  $\langle f \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \rangle_n = f(\mathbf{J}_n)$ . *Proof.* We examine the i, j element of the  $n \times n$  matrix  $f(\mathbf{J}_n)$ .

$$\mathbf{e}_{i}^{T} f(\mathbf{J}_{n}) \mathbf{e}_{j} = \mathbf{e}_{i}^{T} \mathbf{Q}_{n} f(\mathbf{\Lambda}_{n}) \mathbf{Q}_{n}^{T} \mathbf{e}_{j}$$

$$= \mathbf{q}_{i}^{T} f(\mathbf{\Lambda}_{n}) \mathbf{q}_{j}$$

$$= \sum_{k=0}^{n-1} f(\lambda_{k}) \frac{\pi_{i}(\lambda_{k})}{\|\boldsymbol{\pi}(\lambda_{k})\|_{2}} \frac{\pi_{j}(\lambda_{k})}{\|\boldsymbol{\pi}(\lambda_{k})\|_{2}}$$

$$= \sum_{k=0}^{n-1} f(\lambda_{k}) \pi_{i}(\lambda_{k}) \pi_{j}(\lambda_{k}) \nu_{k}^{n}$$

$$= \langle f \pi_{i} \pi_{j} \rangle_{n},$$

which completes the proof.  $\Box$ 

Note that Lemma 4.1 generalizes Theorem 3.4 in [17]. With this in the arsenal, we can prove the following theorem relating pseudospectral to Galerkin.

THEOREM 4.2. The pseudospectral solution is equal to an approximation of the Galerkin solution where each integral in equation (3.28) is approximated by an n-point Gauss quadrature formula. In other words,  $\mathbf{X}_p$  solves

$$\left\langle \boldsymbol{\pi}_{n} \boldsymbol{\pi}_{n}^{T} \otimes A \right\rangle_{n} \operatorname{vec}(\mathbf{X}_{p}) = \left\langle \boldsymbol{\pi}_{n} \otimes \mathbf{b} \right\rangle_{n}.$$
 (4.1)

*Proof.* Define the  $N \times n$  matrix  $\mathbf{B}_c = [b(\lambda_0) \cdots b(\lambda_{n-1})]$ . Using the power series expansion of A(s) (equation (2.3)), we can write the matrix of each collocation solution as

$$A(\lambda_k) = \sum_{i=0}^{\infty} \mathbf{A}_i \lambda_k^i \tag{4.2}$$

for  $k = 0, \ldots, n-1$ . We collect these into one large block-diagonal system by writing

$$\left(\sum_{i=0}^{\infty} \mathbf{\Lambda}_{n}^{i} \otimes \mathbf{A}_{i}\right) \operatorname{vec}(\mathbf{X}_{c}) = \operatorname{vec}(\mathbf{B}_{c}).$$
(4.3)

Let **I** be the  $N \times N$  identity matrix. Premultiply (4.3) by ( $\mathbf{D}_{\mathbf{q}_0} \otimes \mathbf{I}$ ), and by commutativity of diagonal matrices and the mixed product property, it becomes

$$\left(\sum_{i=0}^{\infty} \mathbf{\Lambda}_{n}^{i} \otimes \mathbf{A}_{i}\right) (\mathbf{D}_{\mathbf{q}_{0}} \otimes \mathbf{I}) \operatorname{vec}(\mathbf{X}_{c}) = (\mathbf{D}_{\mathbf{q}_{0}} \otimes \mathbf{I}) \operatorname{vec}(\mathbf{B}_{c}).$$
(4.4)

Premultiplying (4.4) by  $(\mathbf{Q}_n \otimes \mathbf{I})$ , properly inserting  $(\mathbf{Q}_n^T \otimes \mathbf{I})(\mathbf{Q}_n \otimes \mathbf{I})$  on the left hand side, and using the eigenvalue decomposition (3.6), this becomes

$$\left(\sum_{i=0}^{\infty} \mathbf{J}_{n}^{i} \otimes \mathbf{A}_{i}\right) (\mathbf{Q}_{n} \otimes \mathbf{I}) (\mathbf{D}_{\mathbf{q}_{0}} \otimes \mathbf{I}) \operatorname{vec}(\mathbf{X}_{c}) = (\mathbf{Q}_{n} \otimes \mathbf{I}) (\mathbf{D}_{\mathbf{q}_{0}} \otimes \mathbf{I}) \operatorname{vec}(\mathbf{B}_{c}).$$
(4.5)

But note that Lemma 3.1 implies

$$(\mathbf{Q}_n \otimes \mathbf{I})(\mathbf{D}_{\mathbf{q}_0} \otimes \mathbf{I})\operatorname{vec}(\mathbf{X}_c) = \operatorname{vec}(\mathbf{X}_p).$$
(4.6)

Using an argument identical to the proof of Lemma 3.1, we can write

$$(\mathbf{Q}_n \otimes \mathbf{I})(\mathbf{D}_{\mathbf{q}_0} \otimes \mathbf{I}) \operatorname{vec}(\mathbf{B}_c) = \langle \boldsymbol{\pi}_n \otimes \boldsymbol{b} \rangle_n$$
(4.7)

Finally, using Lemma 4.1, equation (4.5) becomes

$$\langle \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \otimes A \rangle_n \operatorname{vec}(\mathbf{X}_p) = \langle \boldsymbol{\pi}_n \otimes b \rangle_n.$$
 (4.8)

as required.

Theorem 4.2 begets a corollary giving conditions for equivalence between Galerkin and pseudospectral approximations.

COROLLARY 4.3. If b(s) contains only polynomials of maximum degree  $m_b$  and A(s) contains only polynomials of maximum degree 1 (i.e. linear functions of s), then  $x_{g,n}(s) = x_{p,n}(s)$  for  $n \ge m_b$  for all  $s \in [-1, 1]$ .

*Proof.* The parameterized matrix  $\pi_n(s)\pi_n(s)^T \otimes A(s)$  has polynomials of degree at most 2n-1. Thus, by the polynomial exactness of the Gauss quadrature formulas,

$$\langle \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \otimes A \rangle_n = \langle \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \otimes A \rangle, \qquad \langle \boldsymbol{\pi}_n \otimes b \rangle_n = \langle \boldsymbol{\pi}_n \otimes b \rangle.$$
 (4.9)

Therefore  $\mathbf{X}_g = \mathbf{X}_p$ , and consequently

$$x_{g,n}(s) = \mathbf{X}_g \boldsymbol{\pi}_n(s) = \mathbf{X}_p \boldsymbol{\pi}_n(s) = x_{p,n}(s).$$
 (4.10)

as required.  $\Box$ 

By taking the transpose of equation (3.27) and following the steps of the proof of theorem 4.2, we get another interesting corollary.

COROLLARY 4.4. First define  $A(\mathbf{J}_n)$  to be the  $Nn \times Nn$  constant matrix with the i, j block of size  $n \times n$  equal to  $A(i, j)(\mathbf{J}_n)$ . Next define  $b(\mathbf{J}_n)$  to be the  $Nn \times n$  constant matrix with the ith  $n \times n$  block equal to  $b_i(\mathbf{J}_n)$ . Then the pseudospectral coefficients  $\mathbf{X}_p$  satisfy

$$A(\mathbf{J}_n)\operatorname{vec}(\mathbf{X}_p^T) = b(\mathbf{J}_n)\mathbf{e}_0, \qquad (4.11)$$

where  $\mathbf{e}_0 = [1, 0, ..., 0]^T$  is an *n*-vector.

Theorem 4.2 leads to a fascinating connection between the matrix operators in the Galerkin and pseudospectral methods, namely that the matrix in the Galerkin system is equal to a submatrix of the matrix from a sufficiently larger pseudospectral computation. This is the key to understanding the relationship between the Galerkin and pseudospectral approximations. In the following lemma, we denote the first  $r \times r$  principal minor of a matrix  $\mathbf{M}$  by  $[\mathbf{M}]_{r \times r}$ .

LEMMA 4.5. Let A(s) contain only polynomials of degree at most  $m_a$ , and let b(s) contain only polynomials of degree at most  $m_b$ . Define

$$m \equiv m(n) \ge \max\left(\left\lceil \frac{m_a + 2n - 1}{2} \right\rceil, \left\lceil \frac{m_b + n}{2} \right\rceil\right)$$
 (4.12)

Then

$$\langle \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \otimes A \rangle = \left[ \langle \boldsymbol{\pi}_m \boldsymbol{\pi}_m^T \otimes A \rangle_m \right]_{Nn \times Nn} \langle \boldsymbol{\pi}_n \otimes b \rangle = \left[ \langle \boldsymbol{\pi}_m \otimes b \rangle_m \right]_{Nn \times 1}.$$

*Proof.* The integrands of the matrix  $\langle \boldsymbol{\pi}_n \boldsymbol{\pi}_n^T \otimes A \rangle$  are polynomials of degree at most  $2n + m_a - 2$ . Therefore they can be integrated exactly with a Gauss quadrature rule of order m. A similar argument holds for  $\langle \boldsymbol{\pi}_n \otimes b \rangle$ .

Combining Lemma 4.5 with corollary 4.4, we get the following proposition relating the Galerkin coefficients to the Jacobi matrices for A(s) and b(s) that depend polynomially on s.

PROPOSITION 4.6. Let m,  $m_a$ , and  $m_b$  be defined as in Lemma 4.5. Define  $[A]_n(\mathbf{J}_m)$  to be the  $Nn \times Nn$  constant matrix with the i, j block of size  $n \times n$  equal to  $[A(i, j)(\mathbf{J}_m)]_{n \times n}$  for  $i, j = 0, \ldots, N-1$ . Define  $[b]_n(\mathbf{J}_m)$  to be the  $Nn \times n$  constant matrix with the ith  $n \times n$  block equal to  $[b_i(\mathbf{J}_m)]_{n \times n}$  for  $i = 1, \ldots, N$ . Then the Galerkin coefficients  $\mathbf{X}_q$  satisfy

$$[A]_n(\mathbf{J}_m)\operatorname{vec}(\mathbf{X}_q^T) = [b]_n(\mathbf{J}_m)\mathbf{e}_0, \qquad (4.13)$$

where  $\mathbf{e}_0 = [1, 0, ..., 0]^T$  is an *n*-vector.

Notice that Proposition 4.6 provides a way to compute the exact matrix for the Galerkin computation without any symbolic manipulation, but beware that m depends on both n and the largest degree of polynomial in A(s). Written in this form, we have no trouble taking m to infinity, and we arrive at the main theorem of this section.

THEOREM 4.7. Using the notation of Proposition 4.6 and corollary 4.4, the coefficients  $\mathbf{X}_g$  of the n-term Galerkin approximation of the solution x(s) to equation (2.2) satisfy the linear system of equations

$$[A]_n(\mathbf{J}_{\infty})\operatorname{vec}(\mathbf{X}_g^T) = [b]_n(\mathbf{J}_{\infty})\mathbf{e}_0, \qquad (4.14)$$

where  $\mathbf{e}_0 = [1, 0, ..., 0]^T$  is an *n*-vector.

**Proof.** Let  $A^{(m_a)}(s)$  be the truncated power series of A(s) up to order  $m_a$ , and let  $b^{(m_b)}(s)$  be the truncated power series of b(s) up to order  $m_b$ . Since A(s) is analytic and bounded away from singularity for all  $s \in [-1, 1]$ , there exists an integer M such that  $A^{(m_a)}(s)$  is also bounded away from singularity for all  $s \in [-1, 1]$ , and all  $m_a > M$  (although the bound may be depend on  $m_a$ ). Assume that  $m_a > M$ .

Define m as in equation (4.12). Then by Proposition 4.6, the coefficients  $\mathbf{X}_{g}^{(m_{a},m_{b})}$  of the n-term Galerkin approximation to the solution of the truncated system satisfy

$$[A^{(m_a)}]_n(\mathbf{J}_m)\operatorname{vec}((\mathbf{X}_g^{(m_a,m_b)})^T) = [b^{(m_b)}]_n(\mathbf{J}_m)\mathbf{e}_0.$$
(4.15)

By the definition of m (equation (4.12)), equation (4.15) holds for all integers greater than some minimum value. Therefore, we can take  $m \to \infty$  without changing the solution at all, i.e.

$$[A^{(m_a)}]_n(\mathbf{J}_{\infty})\operatorname{vec}((\mathbf{X}_g^{(m_a,m_b)})^T) = [b^{(m_b)}]_n(\mathbf{J}_{\infty})\mathbf{e}_0.$$
(4.16)

Next we take  $m_a, m_b \to \infty$  to get

$$[A^{(m_a)}]_n(\mathbf{J}_{\infty}) \to [A]_n(\mathbf{J}_{\infty})$$
$$[b^{(m_b)}]_n(\mathbf{J}_{\infty}) \to [b]_n(\mathbf{J}_{\infty})$$

which implies

$$\mathbf{X}_{g}^{(m_{a},m_{b})} \to \mathbf{X}_{g} \tag{4.17}$$

as required.  $\Box$ 

Theorem 4.7 and corollary 4.4 reveal the fundamental difference between the Galerkin and pseudospectral approximations. We put them side-by-side for comparison.

$$[A]_n(\mathbf{J}_{\infty})\operatorname{vec}(\mathbf{X}_g^T) = b_n(\mathbf{J}_{\infty})\mathbf{e}_0, \qquad A(\mathbf{J}_n)\operatorname{vec}(\mathbf{X}_p^T) = b(\mathbf{J}_n)\mathbf{e}_0.$$
(4.18)

The difference lies in where the truncation occurs. For pseudospectral, the infinite Jacobi matrix is first truncated, and then the operator is applied. For Galerkin, the operator is applied to the infinite Jacobi matrix, and the resulting system is truncated. The question that remains is whether it matters. As we will see in the error estimates in the next section, the interpolating pseudospectral approximation converges at a rate comparable to the Galerkin approximation, yet requires considerably less computational effort.

5. Error Estimates. Asymptotic error estimates for polynomial approximation are well-established in many contexts, and the theory is now considered classical. Our goal is to apply the classical theory to relate the rate of geometric convergence to some measure of singularity for the solution. We do not seek the tightest bounds in the most appropriate norm as in [6], but instead we offer intuition for understanding the asymptotic rate of convergence. We also present a residual error estimate that may be more useful in practice. We complement the analysis with two representative numerical examples.

To discuss convergence, we need to choose a norm. In the statements and proofs, we will use the standard  $L^2$  and  $L^{\infty}$  norms generalized to  $\mathbb{R}^N$ -valued functions.

DEFINITION 5.1. For a function  $f : \mathbb{R} \to \mathbb{R}^N$ , define the  $L^2$  and  $L^{\infty}$  norms as

$$\|f\|_{L^2} := \sqrt{\sum_{i=0}^{N-1} \int_{-1}^{1} f_i^2(s) w(s) \, ds}$$
(5.1)

$$\|f\|_{L^{\infty}} := \max_{0 \le i \le N-1} \left( \sup_{-1 \le s \le 1} |f_i(s)| \right)$$
(5.2)

With these norms, we can state error estimates for both Galerkin and pseudospectral methods.

THEOREM 5.2 (Galerkin Asymptotic Error Estimate). Let  $\rho^*$  be the sum of the semi-axes of the greatest ellipse with foci at  $\pm 1$  in which  $x_i(s)$  is analytic for  $i = 0, \ldots, N-1$ . Then for  $1 < \rho < \rho^*$ , the asymptotic error in the Galerkin approximation is

$$\|x - x_{g,n}\|_{L^2} \le C\rho^{-n},\tag{5.3}$$

where C is a constant independent of n.

*Proof.* We begin with the standard error estimate for the Galerkin method [6, Section 6.4] in the  $L^2$  norm,

$$\|x - x_{g,n}\|_{L^2} \le C \|x - R_n x\|_{L^2}.$$
(5.4)

The constant C is independent of n but depends on the extremes of the bounded eigenvalues of A(s). Under the consistency hypothesis, the operator  $R_n$  is a projection operator such that

$$\|x_i - R_n x_i\|_{L^2} \to 0, \qquad n \to \infty.$$

$$(5.5)$$

for i = 0, ..., N - 1. For our purpose, we let  $R_n x$  be the expansion of x(s) in terms of the Chebyshev polynomials,

$$R_n x(s) = \sum_{k=0}^{n-1} \mathbf{a}_k T_k(s),$$
(5.6)

where  $T_k(s)$  is the kth Chebyshev polynomial, and

$$\mathbf{a}_{k,i} = \frac{2}{\pi c_k} \int_{-1}^{1} x_i(s) T_k(s) (1-s^2)^{-1/2} \, ds, \qquad c_k = \begin{cases} 2 & \text{if } k = 0\\ 1 & \text{otherwise} \end{cases}$$
(5.7)

for i = 0, ..., N-1. Since x(s) is continuous for all  $s \in [-1, 1]$  and w(s) is normalized, we can bound

$$\|x - R_n x\|_{L^2} \le \sqrt{N} \|x - R_n x\|_{L^{\infty}}$$
(5.8)

The Chebyshev series converges uniformly for functions that are continuous on [-1, 1], so we can bound

$$\|x - R_n x\|_{L^{\infty}} = \left\|\sum_{k=n}^{\infty} \mathbf{a}_k T_k(s)\right\|_{L^{\infty}}$$

$$(5.9)$$

$$\leq \left\|\sum_{k=n}^{\infty} |\mathbf{a}_k|\right\|_{\infty} \tag{5.10}$$

since  $-1 \leq T_k(s) \leq 1$  for all k. To be sure, the quantity  $|\mathbf{a}_k|$  is the component-wise absolute value of the constant vector  $\mathbf{a}_k$ , and the norm  $\|\cdot\|_{\infty}$  is the standard infinity norm on  $\mathbb{R}^N$ .

Using the classical result stated in [19, Section 3], we have

$$\limsup_{k \to \infty} |\mathbf{a}_{k,i}|^{1/k} = \frac{1}{\rho_i^*}, \qquad i = 0, \dots, N-1$$
(5.11)

where  $\rho_i^*$  is the sum of the semi-axes of the greatest ellipse with foci at  $\pm 1$  in which  $x_i(s)$  is analytic. This implies that asymptotically

$$|\mathbf{a}_{k,i}| = \mathcal{O}\left(\frac{\rho_i}{k}\right), \qquad i = 0, \dots, N-1.$$
(5.12)

for  $\rho_i < \rho_i^*$ . We take  $\rho = \min_i \rho_i$ , which suffices to prove the estimate (5.3).

Theorem 5.2 recalls the well-known fact that the convergence of many polynomial approximations (e.g. power series, Fourier series) depend on the size of the region in the complex plane in which the function is analytic. Thus, the location of the singularity nearest the interval [-1, 1] determines the rate at which the approximation converges as one includes higher powers in the polynomial approximation. Next we derive a similar result for the pseudospectral approximation using the fact that it interpolates x(s) at the Gauss points of the weight function w(s).

THEOREM 5.3 (Pseudospectral Asymptotic Error Estimate). Let  $\rho^*$  be the sum of the semi-axes of the greatest ellipse with foci at  $\pm 1$  in which  $x_i(s)$  is analytic for  $i = 0, \ldots, N - 1$ . Then for  $1 < \rho < \rho^*$ , the asymptotic error in the pseudospectral approximation is

$$\|x - x_{p,n}\|_{L^2} \le C\rho^{-n},\tag{5.13}$$

where C is a constant independent of n.

*Proof.* Recall that  $x_{c,n}(s)$  is the Lagrange interpolant of x(s) at the Gauss points of w(s), and let  $x_{c,n,i}(s)$  be the *i*th component of  $x_{c,n}(s)$ . We will use the result from [25, Theorem 4.8] that

$$\int_{-1}^{1} (x_i(s) - x_{c,n,i}(s))^2 w(s) \, ds \le 4E_n^2(x_i), \tag{5.14}$$

where  $E_n(x_i)$  is the error of the best approximation polynomial in the uniform norm. We can, again, bound  $E_n(x_i)$  by the error of the Chebyshev expansion (5.6). Using Theorem 3.2 with equation (5.14),

$$\begin{aligned} \|x - x_{p,n}\|_{L^2} &= \|x - x_{c,n}\|_{L^2} \\ &\leq 2\sqrt{N} \|x - R_n x\|_{L^{\infty}} \end{aligned}$$

The remainder of the proof proceeds exactly as the proof of theorem 5.2.  $\Box$ 

We have shown, using classical approximation theory, that the interpolating pseudospectral method and the Galerkin method have the same asymptotic rate of geometric convergence. This rate of convergence depends on the size of the region in the complex plane where the functions x(s) are analytic. The structure of the matrix equation reveals at least one singularity that occurs when  $A(s^*)$  is rank-deficient for some  $s^* \in \mathbb{R}$ , assuming the right hand side  $b(s^*)$  does not fortuitously remove it. For a general parameterized matrix, this fact may not be useful. However, for many parameterized systems in practice, the range of the parameter is dictated by existence and/or stability criteria. The value that makes the system singular is often known and has some interpretation in terms of the model. In these cases, one may have an upper bound on  $\rho$ , which is the sum of the semi-axes of the ellipse of analyticity, and this can be used to estimate the geometric rate of convergence *a priori*.

We end this section with a residual error estimate – similar to residual error estimates for constant matrix equations – that may be more useful in practice than the asymptotic results.

THEOREM 5.4. Define the residual r(y, s) as in equation (3.22), and let e(y, s) = x(s) - y(s) be the  $\mathbb{R}^N$ -valued function representing the error in the approximation y(s). Then

$$C_1 \|r(y)\|_{L^2} \le \|e(y)\|_{L^2} \le C_2 \|r(y)\|_{L^2}$$
(5.15)

for some constants  $C_1$  and  $C_2$ , which are independent of y(s).

*Proof.* Since A(s) is non-singular for all  $s \in [-1, 1]$ , we can write

$$A^{-1}(s)r(y,s) = y(s) - A^{-1}(s)b(s) = e(y,s)$$
(5.16)

so that

$$\begin{aligned} \|e(y)\|_{L^2}^2 &= \left\langle e(y)^T e(y) \right\rangle \\ &= \left\langle r^T(y) A^{-T} A^{-1} r(y) \right\rangle \end{aligned}$$

Since A(s) is bounded, so is  $A^{-1}(s)$ . Therefore, there exist constants  $C_1^*$  and  $C_2^*$  that depend only on A(s) such that

$$C_1^* \left\langle r^T(y) r(y) \right\rangle \le \left\langle e^T(y) e(y) \right\rangle \le C_2^* \left\langle r^T(y) r(y) \right\rangle.$$
(5.17)

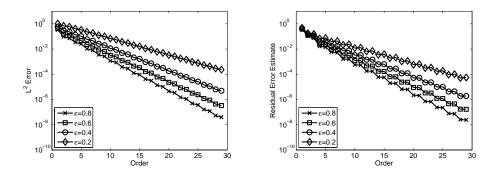


FIG. 6.1. The convergence of the spectral methods applied to equation (6.1). The figure on the left shows plots the  $L^2$  error as the order of approximation increases, and the figure on the right plots the residual error estimate. The stairstep behavior relates to the fact that  $x_0(s)$  and  $x_1(s)$  are odd functions over [-1, 1].

Taking the square root yields the desired result.  $\Box$ 

Theorem 5.4 states that the  $L^2$  norm of the residual behaves like the  $L^2$  norm of the error. In many cases, this residual error may be much easier to compute than the true  $L^2$  error. However, as in residual error estimates for constant matrix problems, the constants in Theorem 5.4 will be large if the bounds on the eigenvalues of A(s)are large. We apply these results in the next section with two numerical examples.

6. Numerical Examples. We examine two simple examples of spectral methods applied to parameterized matrix equations. The first is a  $2 \times 2$  symmetric parameterized matrix, and the second comes from a discretized second order ODE. In both cases, we relate the convergence of the spectral methods to the size of the region of analyticity and verify this relationship numerically. We also compare the behavior of the true error to the behavior of the residual error estimate from theorem 5.4.

To keep the computations simple, we use a constant weight function w(s). The corresponding orthonormal polynomials are the normalized Legendre polynomials, and the Gauss points are the Gauss-Legendre points.

6.1. A 2 × 2 Parameterized Matrix Equation. Let  $\epsilon > 0$ , and consider the following parameterized matrix equation

$$\begin{bmatrix} 1+\varepsilon & s\\ s & 1 \end{bmatrix} \begin{bmatrix} x_0(s)\\ x_1(s) \end{bmatrix} = \begin{bmatrix} 2\\ 1 \end{bmatrix}.$$
 (6.1)

For this case, we can easily compute the exact solution,

$$x_0(s) = \frac{2-s}{1+\varepsilon - s^2}, \qquad x_1(s) = \frac{1+\varepsilon - 2s}{1+\varepsilon - s^2}.$$
(6.2)

Both of these functions have a poles at  $s = \pm \sqrt{1 + \varepsilon}$ , so the sum of the semi-axes of the ellipse of analyticity is bounded, i.e.  $\rho < \sqrt{1 + \varepsilon}$ . Notice that the matrix is linear in *s*, and the right hand side has no dependence on *s*. Thus, corollary 4.3 implies that the Galerkin approximation is equal to the pseudospectral approximation for all *n*; there is no need to solve the system (3.28) to compute the Galerkin approximation. In figure 6.1 we plot both the true  $L^2$  error and the residual error estimate for four values of  $\varepsilon$ . The results confirm the analysis.

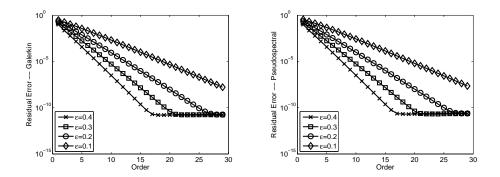


FIG. 6.2. The convergence of the residual error estimate for the Galerkin and pseudospectral approximations applied to the parameterized matrix equation (6.8).

**6.2.** A Parameterized Second Order ODE. Consider the second order boundary value problem

$$\frac{d}{dt}\left(\alpha(s,t)\frac{du}{dt}\right) = 1 \qquad t \in [0,1]$$
(6.3)

$$u(0) = 0 \tag{6.4}$$

$$u(1) = 0$$
 (6.5)

where, for  $\varepsilon > 0$ ,

$$\alpha(s,t) = 1 + 4\cos(\pi s)(t^2 - t), \qquad s \in [\varepsilon, 1].$$
 (6.6)

The exact solution is

$$u(s,t) = \frac{1}{8\cos(\pi s)} \ln\left(1 + 4\cos(\pi s)(t^2 - t)\right).$$
(6.7)

The solution u(s,t) has a singularity at s = 0 and t = 1/2. Notice that we have adjusted the range of s to be bounded away from 0 by  $\varepsilon$ . We use a standard piecewise linear Galerkin finite element method with 512 elements in the t domain to construct a stiffness matrix parameterized by s, i.e.

$$(K_0 + \cos(\pi s)K_1)x(s) = b.$$
(6.8)

Figure 6.2 shows the convergence of the residual error estimate for both Galerkin and pseudospectral approximations as n increases. (Despite having the exact solution (6.7) available, we do not present the decay of the  $L^2$  error; it is dominated entirely by the discretization error in the t domain.) As  $\varepsilon$  gets closer to zero, the geometric convergence rate of the spectral methods degrades considerably. Also, note that each element of the parameterized stiffness matrix is an analytic function of s, but figure 6.2 verifies that the less expensive pseudospectral approximation converges at the same rate as the Galerkin approximation.

7. Summary and Conclusions. We have presented an application of spectral methods to parameterized matrix equations. Such parameterized systems arise in many applications. The goal of a spectral method is to construct a global polynomial approximation of the  $\mathbb{R}^N$ -valued function that satisfies the parameterized system.

We derived two basic spectral methods: (i) the interpolatory pseudospectral method, which approximates the coefficients of the truncated Fourier series with Gauss quadrature formulas, and (ii) the Galerkin method, which finds an approximation in a finite dimensional subspace by requiring that the equation residual be orthogonal to the approximation space. The primary work involved in the pseudospectral method is solving the parameterized system at a finite set of parameter values, whereas the Galerkin method requires the solution of a coupled system of equations many times larger than the original parameterized system.

We showed that one can interpret the differences between these two methods as a choice of when to truncate an infinite linear system of equations. Employing this relationship we derived conditions under which these two approximations are equivalent. In this case, there is no reason to solve the large coupled system of equations for the Galerkin approximation.

Using classical techniques, we presented asymptotic error estimates relating the decay of the error to the size of the region of analyticity of the solution; we also derived a residual error estimate that may be more useful in practice. We verified the theoretical developments with two numerical examples: a  $2 \times 2$  matrix equation and a finite element discretization of a parameterized second order ODE.

The popularity of spectral methods for PDEs stems from their *infinite* (i.e. geometric) order of convergence for smooth functions compared to finite difference schemes. We have the same advantage in the case of parameterized matrix equations, plus the added bonus that there are no boundary conditions to consider. The primary concern for these methods is determining the value of the parameter closest to the domain that renders the system singular.

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## REFERENCES

- I. BABUŠKA, F. NOBILE, AND R. TEMPONE, A stochastic collocation method for elliptic partial differential equations with random input data, SIAM Journal of Numerical Analysis, 45 (2007), pp. 1005 – 1034.
- [2] I. BABUŠKA, R. TEMPONE, AND G. E. ZOURARIS, Galerkin finite element approximations of stochastic elliptic partial differential equations, SIAM Journal of Numerical Analysis, 42 (2004), pp. 800 – 825.
- [3] J. P. BOYD, Chebyshev and Fourier Spectral Methods, Dover, 2nd ed., 2001.
- [4] S. C. BRENNER AND L. R. SCOTT, The Mathematical Theory of Finite Element Methods, Springer, 2nd ed., 2002.
- [5] C. BREZINSKI AND M. REDIVO-ZAGLIA, The PageRank vector: Properties, computation, approximation, and acceleration, SIAM Journal on Matrix Analysis and Applications, 28 (2006), pp. 551–575.
- [6] C. CANUTO, M. Y. HUSSAINI, A. QUARTERONI, AND T. A. ZANG, Spectral Methods: Fundamentals in Single Domains, Springer, 2006.
- [7] S. CHANDRASEKARAN, G. H. GOLUB, M. GU, AND A. H. SAYED, Parameter estimation in the presence of bounded data uncertainties, SIAM Journal on Matrix Analysis and Applications, 19 (1998), pp. 235–252.
- [8] J. CHUNG AND J. G. NAGY, Nonlinear least squares and super resolution, Journal of Physics: Conference Series, 124 (2008), p. 012019 (10pp).
- [9] P. G. CONSTANTINE AND D. F. GLEICH, Using polynomial chaos to compute the influence of multiple random surfers in the PageRank model, in Proceedings of the 5th Workshop on Algorithms and Models for the Web Graph, Springer, ed., 2007.

- [10] L. DIECI AND L. LOPEZ, Lyapunov exponents of systems evolving on quadratic groups, SIAM Journal on Matrix Analysis and Applications, 24 (2003), pp. 1175–1185.
- [11] H. C. ELMAN, O. G. ERNST, D. P. O'LEARY, AND M. STEWART, Efficient iterative algorithms for the stochastic finite element method with application to acoustic scattering, Computer Methods in Applied Mechanics and Engineering, 194 (2005), pp. 1037 – 1055.
- [12] O. ERNST, C. POWELL, D. SILVESTER, AND E. ULLMANN, Efficient solvers for a linear stochastic Galerkin mixed formulation of diffusion problems with random data, SIAM Journal on Scientific Computing, 31 (2009), pp. 1424–1447.
- [13] P. FRAUENFELDER, C. SCHWAB, AND R. A. TODOR, Finite elements for elliptic problems with stochastic coefficients, Computer Methods in Applied Mechanics and Engineering, 194 (2005), pp. 205 – 228. Selected papers from the 11th Conference on The Mathematics of Finite Elements and Applications.
- [14] W. GAUTSCHI, The interplay between classical analyses and (numerical) linear algebra a tribute to Gene Golub, Electronic Transactions on Numerical Analysis, 13 (2002), pp. 119 – 147.
- [15] , Orthogonal Polynomials: Computation and Approximation, Clarendon Press, Oxford, 2004.
- [16] R. GHANEM AND P. SPANOS, Stochastic Finite Elements: A Spectral Approach, Springer-Verlag, New York, 1991.
- [17] G. H. GOLUB AND G. MEURANT, Matrices, moments, and quadrature, Longman, Essex, U.K., 1994.
- [18] G. H. GOLUB AND C. F. VANLOAN, Matrix Computations, The Johns Hopkins University Press, Baltimore, MD, 3rd ed., 1996.
- [19] D. GOTTLIEB AND S. A. ORSZAG, Numerical Analysis of Spectral Methods: Theory and Applications, SIAM, 1977.
- [20] J. S. HESTHAVEN, S. GOTTLIEB, AND D. GOTTLIEB, Spectral Methods for Time Dependent Problems, Cambridge University Press, 2007.
- [21] T. KATO, Perturbation Theory for Linear Operators, Springer-Verlag, 2nd ed., 1980.
- [22] Y.-T. LI, Z. BAI, AND Y. SU, A two-directional Arnoldi process and its application to parametric model order reduction, Journal of Computational and Applied Mathematics, 226 (2009), pp. 10 – 21. Special Issue: The First International Conference on Numerical Algebra and Scientific Computing (NASC06).
- [23] C. D. MEYER, Matrix Analysis and Applied Linear Algebra, SIAM, 2000.
- [24] C. E. POWELL AND H. C. ELMAN, Block-diagonal preconditioning for spectral stochastic finiteelement systems, IMA Journal of Numerical Analysis, Advance Access, (2008).
- [25] T. J. RIVLIN, An Introduction to the Approximation of Functions, Blaisdell Publishing Company, 1969.
- [26] G. SZEGÖ, Orthogonal Polynomials, American Mathematical Society, Providence, RI, 1939.
- [27] Q. WANG, P. MOIN, AND G. IACCARINO, A rational interpolation scheme with super-polynomial rate of convergence, (2008), pp. 31–54.
- [28] D. XIU AND J. S. HESTHAVEN, High order collocation methods for differential equations with random inputs, SIAM Journal of Scientific Computing, 27 (2005), pp. 1118 – 1139.
- [29] D. XIU AND G. KARNIADAKIS, The Wiener-Askey polynomial chaos for stochastic differential equations, SIAM Journal of Scientific Computing, 24 (2002), pp. 619 – 644.