STABLE EXTRAPOLATION OF ANALYTIC FUNCTIONS

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Abstract. This paper examines the problem of extrapolation of an analytic function for $x > 1$ given perturbed samples from an equally spaced grid on $[-1, 1]$. Mathematical folklore states that extrapolation is in general hopelessly ill-conditioned, but we show that a more precise statement carries an interesting nuance. For a function f on $[-1, 1]$ that is analytic in a Bernstein ellipse with parameter $\rho > 1$, and for a uniform perturbation level ε on the function samples, we construct an asymptotically best extrapolant $e(x)$ as a least squares polynomial approximant of degree M^* given explicitly. We show that the extrapolant $e(x)$ converges to $f(x)$ pointwise in the interval $I_\rho \in [1, (\rho+\rho^{-1})/2)$ as $\varepsilon \to 0$, at a rate given by a x-dependent fractional power of ε. More precisely, for each $x \in I_\rho$ we have

$$|f(x) - e(x)| = \mathcal{O}\left(\varepsilon^{-\log r(x)/\log\rho}\right), \qquad r(x) = \frac{x + \sqrt{x^2-1}}{\rho},$$

up to log factors, provided that the oversampling conditioning is satisfied. That is,

$$M^* \le \frac{1}{2}\sqrt{N},$$

which is known to be needed from approximation theory. In short, extrapolation enjoys a weak form of stability, up to a fraction of the characteristic smoothness length. The number of function samples, $N + 1$, does not bear on the size of the extrapolation error provided that it obeys the oversampling condition. We also show that one cannot construct an asymptotically more accurate extrapolant from $N + 1$ equally spaced samples than $e(x)$, using any other linear or nonlinear procedure. The proofs involve original statements on the stability of polynomial approximation in the Chebyshev basis from equally spaced samples and these are expected to be of independent interest.

Key words. extrapolation, interpolation, Chebyshev polynomials, Legendre polynomials, approximation theory

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1. Introduction. Stable extrapolation is a topic that has traditionally been avoided in numerical analysis, perhaps out of a concern that positive results may be too weak to be interesting. The thorough development of approximation theory for ℓ_1 minimization over the past ten years; however, has led to the discovery of new regimes where *interpolation* of smooth functions is accurate, under a strong assumption of Fourier sparsity [10]. More recently, these results have been extended to deal with the *extrapolation* case, under the name super-resolution [11, 16]. This paper seeks to bridge the gap between these results and traditional numerical analysis, by rolling back the Fourier-sparse assumption and establishing tight statements on the accuracy of extrapolation under the basic assumption that the function is analytic and imperfectly known at equally spaced samples.

1.1. Setup. A function $f : [-1, 1] \to \mathbb{C}$ is real-analytic when each of its Taylor expansions, centered at each point x, converges in a disk of radius $R > 0$. While the parameter R is one possible measure of the smoothness of f, we prefer in this paper to consider the largest Bernstein ellipse, in the complex plane, to which f can be analytically continued. We say that a function $f : [-1, 1] \to \mathbb{C}$ is *analytic with a Bernstein parameter* $\rho > 1$ if it is analytically continuable to a function that is analytic in the open ellipse with foci at ± 1, semiminor and semimajor axis lengths

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summing to ρ, denoted by E_ρ, and bounded in E_ρ so that $|f(z)| \leq Q$ for $z \in E_\rho$ and $Q < \infty$.[1] We denote the set of such functions as $B_\rho(Q)$.

Such a function f has a unique, bounded analytic continuation in the interval $I_\rho = [1, (\rho + \rho^{-1})/2)$, which serves as the reference for measuring the extrapolation error. We denote by $r(x)$, or simply r, the nondimensional length parameter in this interval,

$$r = \frac{x + \sqrt{x^2 - 1}}{\rho},$$

so that $\frac{1}{\rho} \leq r < 1$ for $x \in I_\rho$.

The question we answer in this paper is: "How best to stably extrapolate an analytic function from imperfect equally spaced samples?" More precisely, for known parameters N, ρ, ε, and Q we assume that

- $f \in B_\rho(Q)$;
- $N+1$ imperfect equally spaced function samples of f are given. That is, the vector $f(\underline{x}^{equi}) + \underline{\varepsilon}$ is known, where $\underline{x}^{equi}$ is the vector of $N+1$ equally spaced points on $[-1, 1]$ so that $x_k = 2k/N - 1$ for $0 \leq k \leq N$ and $\underline{\varepsilon}$ is a perturbation vector with $\|\underline{\varepsilon}\|_\infty \leq \varepsilon$; and
- $x \in I_\rho$ is an extrapolation point, where $I_\rho = [1, (\rho + \rho^{-1})/2)$.

Our task is to construct an extrapolant $e(x)$ for $f(x)$ in the interval I_ρ from the imperfect equally spaced samples that minimizes the extrapolation error $|f(x) - e(x)|$ for $x \in I_\rho$.

Extrapolation is far from being the counterpoint to interpolation, and several different ideas are required. First, the polynomial interpolant of an analytic function f at $N+1$ equally spaced points on $[-1, 1]$ can suffer from wild oscillations near ± 1, known as Runge's phenomenon [30]. Second, the construction of an equally spaced polynomial interpolant is known to be exponentially ill-conditioned, leading to practical problems with computations performed in floating point arithmetic. Various remedies are proposed for the aforementioned problems,[2] and in this paper we show that one approach is simply least-squares approximation by polynomials of much lower degree than the number of function samples.

For a given integer $0 \leq M \leq N$, we denote by $p_M(x)$ the least squares polynomial fit of degree M to the imperfect samples, i.e.,

$$p_M = \mathrm{argmin}_{p \in \mathcal{P}_M} \|f(\underline{x}^{equi}) + \underline{\varepsilon} - p(\underline{x}^{equi})\|_2, \tag{1}$$

where $\mathcal{P}_M$ is the space of polynomials of degree at most M. In this paper, we show that a near-best extrapolant $e(x)$ is given by

$$e(x) = p_{M^*}(x), \tag{2}$$

where

$$M^* = \left\lfloor \min\left\{ \frac{1}{2}\sqrt{N}, \frac{\log(Q/\varepsilon)}{\log(\rho)} \right\} \right\rfloor. \tag{3}$$

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[1] The relationship between R and ρ is found by considering f analytic in the so-called stadium of radius $R > 0$, i.e., the region $S_R = \{z \in \mathbb{C} : \inf_{x \in [-1,1]} |z - x| < R\}$. If f is analytic with a Bernstein parameter $\rho > 1$, then f is also analytic in the stadium with radius $R = (\rho + \rho^{-1})/2 - 1$. Conversely, if f is analytic in S_R, then f is analytic with a Bernstein parameter $\rho = R + \sqrt{R^2 + 1}$. See [17, 14] for details.

[2] Among them, least squares polynomial fitting [12], mock Chebyshev interpolation [8], polynomial overfitting with constraints [7], and the Bernstein polynomial basis [27, Sec. 6.3]. For an extensive list, see [26].

Here, $\lfloor a \rfloor$ denotes the largest integer less than or equal to a, but exactly how the integer part is taken in (3) is not particularly important. The formula for M^* in (3) is derived by approximately balancing two terms: a noiseless term that is geometrically decaying to zero with M and a noise term that is exponentially growing with M. It is the exponentially growing noise term that has lead researchers to the conclusion that polynomial extrapolation is unstable in practice. The balance of these two terms roughly minimizes the extrapolation error. If $\log(Q/\varepsilon)/\log(\rho) < \frac{1}{2}\sqrt{N}$, then this balancing can be achieved without violating a necessary oversampling condition; otherwise, $\log(Q/\varepsilon)/\log(\rho) \geq \frac{1}{2}\sqrt{N}$ and one gets as close as possible to the balancing of the two terms by setting $M^* = \frac{1}{2}\sqrt{N}$.

1.2. Main results. The behavior of the extrapolation error depends on whether $M^* = \frac{1}{2}\sqrt{N}$ or not (see (3)), and the two corresponding regimes are referred to as *undersampled* and *oversampled*, respectively.

Definition 1. *The extrapolation problem with parameters $(N, \rho, \varepsilon, Q)$ is said to be oversampled if*

$$\frac{\log(Q/\varepsilon)}{\log(\rho)} < \frac{1}{2}\sqrt{N}. \tag{4}$$

Conversely, if this inequality is not satisfied, then the problem is said to be undersampled.

The relation between M and N stems from the observation that polynomial approximation on an equally spaced grid can be computed stably when $M \leq \frac{1}{2}\sqrt{N}$, as we show in the sequel, but not if M is asymptotically larger than $\sqrt{N}$ [26, p. 3]. In [13] it is empirically observed that (1) can be solved without any numerical issues if $M < 2\sqrt{N}$ and yet another illustration of this relationship is the so-called mock-Chebyshev grid, which is a subset of an $N+1$ equally spaced grid of size $M \sim \sqrt{N}$ that allows for stable polynomial interpolation [8].

We now give one of our main theorems. For convenience, let

$$\alpha(x) = -\frac{\log r(x)}{\log \rho},$$

which is the fractional power of the perturbation level ε in the error bound below.

Theorem 2. *Consider the extrapolation problem with parameters $(N, \rho, \varepsilon, Q)$.*

- *If (4) holds (oversampled case), then for all $x \in I_\rho$,*

$$|f(x) - e(x)| \leq C_{\rho,\varepsilon} \, \frac{Q}{1 - r(x)} \, \left(\frac{\varepsilon}{Q}\right)^{\alpha(x)}, \tag{5}$$

  where $C_{\rho,\varepsilon}$ is a constant that depends polylogarithmically on $1/\varepsilon$.
- *If (4) does not hold (undersampled case), then for all $x \in I_\rho$,*

$$|f(x) - e(x)| \leq C_{\rho,N} \, \frac{Q}{1 - r(x)} \, r(x)^{\frac{1}{2}\sqrt{N}}, \tag{6}$$

  where $C_{\rho,N}$ is a constant that depends polynomially on N.

Note that $\alpha(x)$ is strictly decreasing in $x \in I_\rho$ with $\alpha(1) = 1$ (the error is proportional to ε at $x = 1$, as expected) to $\alpha((\rho + \rho^{-1})/2) = 0$ where the Bernstein ellipse meets the real axis (there is no expectation of control over the extrapolation error at

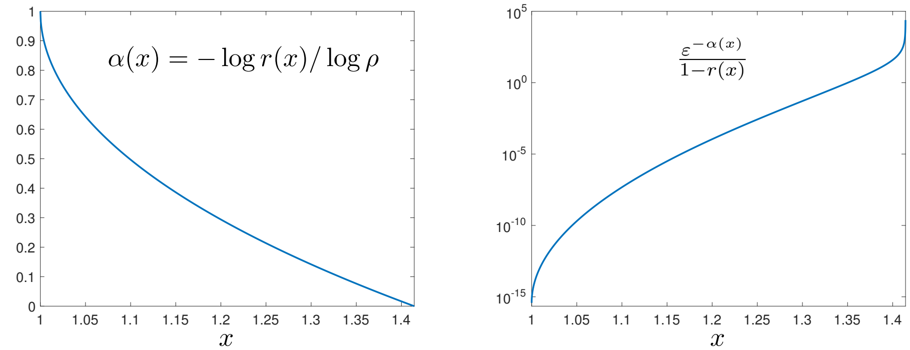

FIG. 1. *In the oversampled case, the near-optimal extrapolant for $f(x)$ in $I_\rho = [1, (\rho+\rho^{-1})/2)$ is given by $e(x) = p_{M^*}(x)$, where $M^* = \lfloor \log(Q/\varepsilon)/\log\rho \rfloor$. The accuracy of extrapolation depends on a fractional power of ε multiplied by $(1-r(x))^{-1}$, i.e., $\varepsilon^{-\alpha(x)}/(1-r(x))$, where $\alpha(x) = \log r(x)/\log\rho$. Here, $\alpha(x)$ (left) and the extrapolation error with the constant (right) is shown for the function $f(x) = 1/(1+x^2)$, with $\rho = 1+\sqrt{2}$ ($f \in B_{\rho'}(Q')$ for any $\rho' < 1+\sqrt{2}$), and $\varepsilon = 2.2 \times 10^{-16}$. In the oversampled case, no linear or nonlinear scheme can provide an asymptotically more accurate extrapolant in general than this bound (see Proposition 3).*

$x = (\rho+\rho^{-1})/2$ since f could be a rational function with a pole outside the Bernstein ellipse). For $1 < x < (\rho+\rho^{-1})/2$, it is surprising that the minimum extrapolation error is not proportional to ε itself, but an x-dependent fractional power of it. Note that the factor $1/(1-r(x))$ also blows up at the endpoint at $x = (\rho+\rho^{-1})/2$. Figure 1 (left) shows the fractional power of ε that is achieved by our extrapolant in the oversampled case and Figure 1 (right) shows the bound in (5) without the constants for extrapolating the function $1/(1+x^2)$ in double precision.

The bound (5) in Theorem 2 cannot be meaningfully improved, as the following proposition shows.

PROPOSITION 3. *Consider the extrapolation problem with parameters $(N, \rho, \varepsilon, Q)$ such that (4) holds. Then, there exists a function $g \in B_{\rho'}(Q')$ for all $\rho' < \rho$ such that*

$$\max_{x\in[-1,1]} |g(x)| \le \varepsilon,$$

and, for $x \in I_\rho$ and some $c_\rho > 0$,

$$|g(x)| \ge c_\rho \, \frac{1}{1-r(x)} \, \varepsilon^{\alpha(x)}.$$

In other words, $g(x)$ is a valid extrapolant to $f(x) = 0$, to within a tolerance of ε on $x \in [-1,1]$, yet it departs from zero at the same asymptotic rate as the upper bound in Theorem 2 for $x > 1$. This means that there is no other linear or nonlinear procedure for constructing an extrapolant from samples on $[-1,1]$ that can do asymptotically better than the extrapolant that we construct in Theorem 2. For example, an extrapolant constructed by Chebyshev interpolation, piecewise polynomials, rational functions, or any other linear or nonlinear procedure cannot deliver an extrapolation error that is better than (5) in any meaningful way.

1.3. Discussion. The number of equally spaced function samples $N+1$ separates two important regimes:

- *Oversampled regime.* If N is sufficiently large that (4) holds, then further refining of the grid does not improve the extrapolation error. In this regime it is the value of ε that dictates the error (5). The problem is essentially one of (deterministic) statistics.

- *Undersampled regime.* If ε is sufficiently small that (4) does not hold, then the accuracy of the extrapolant is mostly blind to the fact that there is a perturbation level at all. In this regime, it is the number of function samples that dictates the error (6). The problem is essentially one of (classical) numerical analysis.

A similar phenomenon appears in the related problem of super-resolution from bandlimited measurements, where it is also the perturbation level of the function samples that determines the recovery error, provided the number of samples is above a certain threshold [15, 16].

In the oversampled case, there exists a perturbation vector for which the actual extrapolation error nearly matches the error bound for the proposed extrapolant $e(x)$ in (2). This implies that $e(x)$ is a *minimax* estimator for $f(x)$, in the sense that it nearly attains the best possible error

$$E_{\mathrm{minmax}}(x) = \inf_{\widehat{e}} \sup_{f,\underline{\varepsilon}} |f(x) - \widehat{e}(x)|,$$

where the infimum is taken over all possible mappings from the perturbed samples to functions of $x \in I_\rho$, and the supremum assumes that $f \in B_\rho(Q)$ and $\|\underline{\varepsilon}\|_\infty \leq \varepsilon$. This paper does not address the question of whether $e(x)$ is also minimax in the undersampled case.

The statement that "the value of N does not matter provided it is sufficiently large" should not be understood as "acquiring more function samples does not matter for extrapolation". The threshold phenomenon is specific to the model of a deterministic perturbation of level ε, which is independent of N. If instead the entries of the perturbation vector $\underline{\varepsilon}$ are modeled as independent and identically distributed Gaussian entries, $\mathcal{N}(0, s^2)$, then the approximation and extrapolation errors include an extra factor $1/\sqrt{N}$, linked to the local averaging implicitly performed in the least-squares polynomial fits. In this case the extrapolant converges pointwise to f as $N \to \infty$, though only at the so-called parametric rate expected from statistics, not at the subexponential rate (6) expected from numerical analysis (see Section 6.2).

1.4. Auxiliary results of independent interest. Before we can begin to analyze how to extrapolate analytic functions, we derive results regarding the conditioning and approximation power of least squares approximation as well as its robustness to perturbed function samples. These results become useful in Section 6 for understanding how to do extrapolation successfully.

Our auxiliary results may be independent interest so we summarize them here:

- Theorem 7: The condition number of the rectangular $(N+1) \times (M+1)$ Legendre–Vandermonde matrix at equally spaced points (see (15)) with $M \leq \frac{1}{2}\sqrt{N}$ is bounded by $\sqrt{5(2M+1)}$.
- Theorem 8: The condition number of the rectangular $(N+1) \times (M+1)$ Chebyshev–Vandermonde matrix at equally spaced points (see (9)) with $M \leq \frac{1}{2}\sqrt{N}$ is bounded by $\sqrt{375(2M+1)/2}$.
- Theorem 9: When $M \leq \frac{1}{2}\sqrt{N}$, $\|f - p_M\|_\infty = \sup_{x \in [-1,1]} |f(x) - p_M(x)|$ converges geometrically to zero as $M \to \infty$.
- Corollary 11: When $M \leq \frac{1}{2}\sqrt{N}$ is fixed and the function samples from f are perturbed by Gaussian noise with a variance of s^2, the expectation of $\|f - p_M\|_\infty$ converges to zero as $N \to \infty$ like $\mathcal{O}(s/\sqrt{N})$.
- Theorem 13: When $M \leq \frac{1}{2}\sqrt{N}$ and the function samples are noiseless the extrap-

olation error $|f(x) - p_M(x)|$ for each $x \in I_\rho$ converges geometrically to zero as $M \to \infty$.

- Corollary 14: If one exponentially oversamples on $[-1,1]$, i.e., $M \leq c\log(N)$ for a small constant c and the function samples are perturbed by Gaussian noise, then $|f(x) - p_M(x)|$ converges to zero as $M \to \infty$ for each $x \in I_\rho$.

Note that Theorem 9 shows that the convergence of $p_M(x)$ is geometrically fast with respect to M, but subexponential with respect in N when $M = \lfloor \frac{1}{2}\sqrt{N} \rfloor$. One cannot achieve a better convergence rate with respect to N by using any other stable linear or nonlinear approximation scheme based on equally spaced function samples [26].

Readers familiar with the paper by Adcock and Hansen [1], which shows how to stably recover functions from its Fourier coefficients may consider Section 3 and Section 4 as a discrete and nonperiodic analogue of their work. Related work based on Fourier expansions, includes the recovery of piecewise analytic functions from Fourier modes [2] and a detailed analysis of the stability barrier in [3].

1.5. Notation and background material. The polynomial $p_M(x)$ in (1) can be represented in any polynomial basis for $\mathcal{P}_M$. We use the Chebyshev polynomial basis because it is convenient for practical computations. That is, we express $p_M(x)$ in a Chebyshev expansion given by

$$p_M(x) = \sum_{k=0}^{M} c_k^{cheb} T_k(x), \qquad T_k(x) = \cos(k \cos^{-1} x), \qquad x \in [-1,1], \tag{7}$$

where T_k is the Chebyshev polynomial of degree k, and we seek the vector of Chebyshev coefficients $\underline{c}^{cheb} = (c_0^{cheb}, \ldots, c_M^{cheb})^T$ so that $p_M(x)$ minimizes the ℓ_2-norm in (1).

The vector of Chebyshev coefficients $\underline{c}^{cheb}$ for $p_M(x)$ in (1) satisfies the so-called *normal equations* [22, Alg. 5.3.1] written as

$$\mathbf{T}_M(\underline{x}^{equi})^* \mathbf{T}_M(\underline{x}^{equi}) \underline{c}^{cheb} = \mathbf{T}_M(\underline{x}^{equi})^* \left(\underline{f} + \underline{\varepsilon} \right), \tag{8}$$

where $\underline{f} = f(\underline{x}^{equi})$ is the vector of equally spaced samples and $\mathbf{T}_M(\underline{x}^{equi})$ denotes the $(N+1) \times (M+1)$ Chebyshev–Vandermonde[3] matrix,

$$\mathbf{T}_M(\underline{x}^{equi}) = \begin{bmatrix} T_0(x_0^{equi}) & \cdots & T_M(x_0^{equi}) \\ \vdots & \ddots & \vdots \\ T_0(x_N^{equi}) & \cdots & T_M(x_N^{equi}) \end{bmatrix}. \tag{9}$$

This converts (1) into a routine linear algebra task that can be solved by Gaussian elimination and hence, the computation of $p_M(x)$ in (1) is simple.

If f is analytic with a Bernstein parameter ρ, then f has a Chebyshev expansion $f(x) = \sum_{n=0}^{\infty} a_n^{cheb} T_n(x)$ for $x \in [-1,1]$ with coefficients that decay geometrically to zero as $n \to \infty$.

PROPOSITION 4. *Let f be analytic with a Bernstein parameter $\rho > 1$ and $Q < \infty$. Then, there are coefficients a_n^{cheb} for $n \geq 0$ such that*

- *$f(x) = \sum_{n=0}^{\infty} a_n^{cheb} T_n(x)$, where the series converges uniformly and absolutely to f,*
- *$|a_0^{cheb}| \leq Q$ and $|a_n^{cheb}| \leq 2Q\rho^{-n}$ for $n \geq 1$, and*

[3]The Chebyshev–Vandermonde matrix in (9) is the same as the familiar Vandermonde matrix except the monomials are replaced by Chebyshev polynomials.

- $\sup_{x\in[-1,1]} |f(x) - f_N(x)| \leq 2Q\rho^{-N}/(\rho-1)$, *where* $f_N(x) = \sum_{n=0}^{N} a_n^{cheb} T_n(x)$ *and* $N \geq 0$.

Proof. See [34, Thm. 8.1] and [34, Thm. 8.2]. ∎

Proposition 4 says that the degree N polynomial f_N, constructed by truncating the Chebyshev expansion of f, converges geometrically to f. In general, one cannot expect faster convergence for polynomial approximants of analytic functions. However, it is rare in practical applications for the Chebyshev expansion of f to be known in advance. Instead, one usually attempts to emulate the degree N polynomial f_N by a polynomial interpolant constructed from $N+1$ samples of f. When the samples are taken from Chebyshev points or Gauss–Legendre nodes on $[-1,1]$ a polynomial interpolant can be constructed in a fast and stable manner [18, 24]. The same cannot be said for equally spaced samples on $[-1,1]$ [26]. In this paper we explore the least squares polynomial approximation as a practical alternative to polynomial interpolation when equally spaced samples are known.

For the convenience of the reader we summarize our main notation in Table 1.

1.6. Structure of the paper. The paper is structured as follows. In Section 2 we further investigate the exponential ill-conditioning associated to polynomial interpolation. In Section 3 we show that the normal equations associated with (1) are well-conditioned. In Section 4 we prove that for analytic functions the least squares polynomial fit is asymptotically optimal for a well-conditioned linear approximation scheme when $M \leq \frac{1}{2}\sqrt{N}$ and in Section 5 we show that it is also robust to noisy function samples. In Section 6 we show that the solution $p_M(x)$ from (1) can be used to extrapolate outside of $[-1,1]$ if significant care is taken and we construct the asymptotically best extrapolant $e(x)$ as a polynomial. Finally, in Section 7 we describe a direct algorithm for solving (1) in $\mathcal{O}(M^3 + MN)$ operations based on Toeplitz and Hankel matrices.

2. How bad is equally spaced polynomial interpolation?.

First, we explore how bad equally spaced polynomial interpolation is in practice by taking $M = N$ in (1) and showing that the condition number of the $(N+1)\times(N+1)$ Chebyshev–Vandermonde matrix $\mathbf{T}_N(\underline{x}^{equi})$ in (9) grows exponentially with N.

When $M = N$ the polynomial $p_M(x)$ that minimizes the ℓ_2-norm in (1) also interpolates f at $\underline{x}^{equi}$ and the vector of Chebyshev coefficients $\underline{c}^{cheb}$ for $p_M(x)$ in (7) satisfies the linear system

$$\mathbf{T}_N(\underline{x}^{equi})\underline{c}^{cheb} = \left(\underline{f} + \underline{\varepsilon}\right). \tag{10}$$

By the Lagrange interpolation theorem, $\mathbf{T}_N(\underline{x}^{equi})$ is invertible and mathematically there is a unique solution vector $\underline{c}^{cheb}$ to (10). Unfortunately, it turns out that $\mathbf{T}_N(\underline{x}^{equi})$ is exponentially close to being singular and the vector $\underline{c}^{cheb}$ is far too sensitive to the perturbations in $\underline{f} + \underline{\varepsilon}$ for (10) to be of practical use when N is large.

We explain why the condition number of $\mathbf{T}_N(\underline{x}^{equi})$ grows exponentially with N by relating it to the poorly behaved *Lebesgue constant* of $\underline{x}^{equi}$.

Definition 5 (Lebesgue constant). *Let $x_0,\ldots,x_N$ be a set of $N+1$ distinct points in $[-1,1]$. Then, the Lebesgue constant of $\underline{x} = (x_0,\ldots,x_N)^T$ is defined by*

$$\Lambda_N(\underline{x}) = \sup_{x\in[-1,1]} \sum_{j=0}^{N} |\ell_j(x)|, \qquad \ell_j(x) = \prod_{k=0,k\neq j}^{N} \frac{x-x_k}{x_j-x_k}. \tag{11}$$

Notation	Description
$B_\rho(Q)$	A function f that is analytic in E_ρ and $\lvert f(z)\rvert \leq Q$ for $z \in E_\rho$, where E_ρ is the region enclosed by a ellipse with foci at ± 1 and semimajor and semiminor axis lengths summing to ρ
f	An analytic function on $[-1, 1]$ with Bernstein parameter $\rho > 1$
$N+1$	The number of equally spaced function samples from $[-1, 1]$
M	The desired degree of a polynomial approximation to f
p_M	The least squares polynomial approximation of f, see (1)
$T_k(x)$	Chebyshev polynomial (1st kind) of degree k
$P_k(x)$	Legendre polynomial of degree k
$\underline{x}^{equi}$	Vector of equally spaced points on $[-1, 1]$, i.e., $x_k^{equi} = 2k/N - 1$
$\underline{f}$, $f(\underline{x}^{equi})$	Vector of equally spaced function samples of f
$\underline{\varepsilon}, \varepsilon$	Vector of perturbations in the function samples of f, $\lVert\underline{\varepsilon}\rVert_\infty \leq \varepsilon$
$\mathbf{T}_M(\underline{x})$	The matrix $\begin{bmatrix} T_0(x_0) & \cdots & T_M(x_0) \\ \vdots & \ddots & \vdots \\ T_0(x_N) & \cdots & T_M(x_N) \end{bmatrix} \in \mathbb{R}^{(N+1)\times(M+1)}$
$\Lambda_N(\underline{x})$	Lebesgue constant of $x_0, \ldots, x_N$, see Definition 5
S	Change of basis matrix from Legendre to Chebyshev coefficients $S_{ij} = \begin{cases} \frac{1}{\pi}\Psi\left(\frac{j}{2}\right)^2, & 0 = i \leq j \leq M,\ j \text{ even}, \\ \frac{2}{\pi}\Psi\left(\frac{j-i}{2}\right)\Psi\left(\frac{j+i}{2}\right), & 0 < i \leq j \leq M,\ i+j \text{ even}, \\ 0, & \text{otherwise}, \end{cases}$ where $\Psi(i) = \Gamma(i+1/2)/\Gamma(i+1)$ and $\Gamma(x)$ is the Gamma function
$\sigma_k(A)$	The kth largest singular value of the matrix A
$\kappa_2(A)$	The 2-norm condition number given by $\kappa_2(A) = \lVert A\rVert_2 \lVert A^{-1}\rVert_2$
$\mathcal{N}(\mu, s^2)$	Gaussian distribution with mean μ and variance s^2
$\mathbb{E}[X]$	The expectation of the random variable X

TABLE 1
A summary of our notation.

To experts the fact that $\Lambda_N(\underline{x})$ and the condition number of $\mathbf{T}_N(\underline{x}^{equi})$ are related is not too surprising because polynomial interpolation is a linear approximation scheme [26]. However, the Lebesgue constant $\Lambda_N(\underline{x})$ is usually interpreted as a number that describes how good polynomial interpolation of f at $x_0, \ldots, x_N$ is in comparison to the best minimax polynomial approximation of degree N. That is, the polynomial interpolant of f at $\underline{x}$ is suboptimal by a factor of at most $1 + \Lambda_N(\underline{x})$ [27, p. 24]. Using $\lVert \cdot \rVert_\infty$ to denote the absolute maximum norm of a function on $[-1, 1]$, this can be expressed as

$$\lVert f - p_N \rVert_\infty \leq (1 + \Lambda_N(\underline{x})) \inf_{q \in \mathcal{P}_M} \lVert f - q \rVert_\infty,$$

where p_N is the polynomial of degree at most N such that $p_N(x_k) = f(x_k)$ for $0 \leq k \leq N$. For example, when the interpolation nodes are the Chebyshev points (of the first kind), i.e.,

$$x_k^{cheb} = \cos((k + 1/2)\pi/(N + 1)), \qquad 0 \leq k \leq N, \tag{12}$$

the Lebesgue constant $\Lambda_N(\underline{x}^{cheb})$ grows modestly with N and is bounded by $\frac{2}{\pi}\log(N+1) + 1$ [9]. Thus, the polynomial interpolant of f at $\underline{x}^{cheb}$ is near-best (off by at most a logarithmic factor). In addition, we have[4] $\kappa_2\left(\mathbf{T}_N(\underline{x}^{cheb})\right) = \sqrt{2}$. This means that polynomial interpolants at Chebyshev points are a powerful tool for approximating functions even when polynomial degrees are in the thousands or millions [18].

In stark contrast, the Lebesgue constant for equally spaced points explodes exponentially with N and we have [33, Thm. 2]

$$\frac{2^{N-2}}{N^2} < \Lambda_N(\underline{x}^{equi}) < \frac{2^{N+3}}{N}.$$

Therefore, an equally spaced polynomial interpolant of f can be exponentially worse than the best minimax polynomial approximation of the same degree. Moreover, in Theorem 6 we show that $\kappa_2\left(\mathbf{T}_N(\underline{x}^{equi})\right)$ is related to $\Lambda_N(\underline{x}^{equi})$ and grows at an exponential rate, making practical computations in floating point arithmetic difficult.

THEOREM 6. *Let $\underline{x} = (x_0, \ldots, x_N)$ be a vector of $N+1$ distinct points on $[-1, 1]$. Then,*

$$\Lambda_N(\underline{x}) \leq \kappa_2\left(\mathbf{T}_N(\underline{x})\right) \leq \sqrt{2}(N + 1)\Lambda_N(\underline{x}),$$

where κ_2 is the 2-norm condition number of a matrix, $\Lambda_N(\underline{x})$ is the Lebesgue constant of $\underline{x}$, and $\ell_j(x)$ for $0 \leq j \leq N$ is given in (11).

Proof. The vector $\underline{x}$ contains $N+1$ distinct points so that $\mathbf{T}_N(\underline{x})$ is an invertible matrix. We write $\kappa_2\left(\mathbf{T}_N(\underline{x})\right) = \|\mathbf{T}_N(\underline{x})\|_2\|\mathbf{T}_N(\underline{x})^{-1}\|_2$ and proceed by bounding $\|\mathbf{T}_N(\underline{x})\|_2$ and $\|\mathbf{T}_N(\underline{x})^{-1}\|_2$ separately.

Since $|T_k(x)| \leq 1$ for $k \geq 0$ and $x \in [-1, 1]$, we have $\|\mathbf{T}_N(\underline{x})\|_2 \leq N+1$. To bound $\|\mathbf{T}_N(\underline{x})^{-1}\|_2$ we note that $\mathbf{T}_N(\underline{x}^{cheb})$ is the discrete cosine transform (of type III) [32], where $\underline{x}^{cheb}$ is the vector of Chebyshev points in (12). Hence, $\mathbf{T}_N(\underline{x}^{cheb})D^{-1/2}$ is an orthogonal matrix with $D = \mathrm{diag}(N + 1, (N + 1)/2, \ldots, (N + 1)/2)$. By the Lagrange interpolation formula [27, Sec. 4.1] (applied to each entry of $\mathbf{T}_N(\underline{x})$) we have the following matrix decomposition:

$$\mathbf{T}_N(\underline{x}) = C\mathbf{T}_N(\underline{x}^{cheb}), \qquad C_{ij} = \prod_{k=0,k\neq j}^{N} \frac{x_i - x_k^{cheb}}{x_j^{cheb} - x_k^{cheb}}. \tag{13}$$

Since $\mathbf{T}_N(\underline{x}^{cheb})D^{-1/2}$ is an orthogonal matrix we find that

$$\|\mathbf{T}_N(\underline{x})^{-1}\|_2 = \|D^{-1/2}(\mathbf{T}_N(\underline{x}^{cheb})D^{-1/2})^{-1}C^{-1}\|_2 \leq \sqrt{2}(N + 1)^{-1/2}\|C^{-1}\|_2.$$

We must now bound $\|C^{-1}\|_2$. From (13) we see that C is a generalized Cauchy matrix and hence, there is an explicit formula for its inverse given by [31, Thm. 1]

$$(C^{-1})_{ij} = \prod_{k=0,k\neq j}^{N} \frac{x_i^{cheb} - x_k}{x_j - x_k} := \ell_j(x_i^{cheb}), \qquad 0 \leq i, j \leq N. \tag{14}$$

[4] To show that $\kappa_2\left(\mathbf{T}_N(\underline{x}^{cheb})\right) = \sqrt{2}$, note that $\mathbf{T}_N(\underline{x}^{cheb})$ is the discrete cosine transform (of type III) [32]. Thus, $\mathbf{T}_N(\underline{x}^{cheb})D^{-1/2}$ is an orthogonal matrix with $D = \mathrm{diag}(N + 1, (N + 1)/2, \ldots, (N + 1)/2)$.

By the equivalence of matrix norms, we have $(N+1)^{-1/2}\|C^{-1}\|_\infty \leq \|C^{-1}\|_2 \leq (N+1)^{1/2}\|C^{-1}\|_\infty$ and from (14) we find that

$$\|C^{-1}\|_\infty = \sup_{0\leq i\leq N} \sum_{j=0}^{N} |\ell_j(x_i^{cheb})| \leq \Lambda_N(\underline{x}).$$

The upper bound in the statement of the theorem follows by combining the calculated upper bounds for $\|\mathbf{T}_N(\underline{x})\|_2$ and $\|\mathbf{T}_N(\underline{x})^{-1}\|_2$.

For the lower bound, note that there exists a polynomial p^* of degree N such that $|p(x_k)| \leq 1$ and an $x^* \in [-1,1]$ such that $|p(x^*)| = \Lambda_N(\underline{x})$. Let $p(x) = \sum_{k=0}^{\infty} c_k^{cheb} T_k(x)$. Since $|T_k(x)| \leq 1$ and $|p(x^*)| = \Lambda_N(\underline{x})$, there exists an $0 \leq k \leq N$ such that $|c_k^{cheb}| \geq \Lambda_N(\underline{x})/(N+1)$. Hence, $\|\underline{c}^{cheb}\|_2 \geq \Lambda_N(\underline{x})/(N+1)$ and we have

$$\frac{\Lambda_N(\underline{x})}{N+1} \leq \|\underline{c}^{cheb}\|_2 \leq \|\mathbf{T}_N(\underline{x})^{-1}\|_2 \|p(\underline{x})\|_2 \leq \sqrt{N+1}\|\mathbf{T}_N(\underline{x})^{-1}\|_2.$$

The lower bound in the statement of the theorem follows from $\|\mathbf{T}_N(\underline{x})\|_2 \geq (N+1)^{1/2}\|\mathbf{T}_N(\underline{x})\|_1 \geq (N+1)^{3/2}$. ☐

Theorem 6 explains why $\kappa_2\left(\mathbf{T}_N(\underline{x}^{equi})\right)$ grows exponentially with N and confirms that one should expect severe numerical issues with equally spaced polynomial interpolation, in addition to the possibility of Runge's phenomenon.

It is not the Chebyshev polynomials that should be blamed for the exponential growth of $\kappa_2(\mathbf{T}_N(\underline{x}^{equi}))$ with N, but the equally spaced points on $[-1,1]$. In a different direction, others have focused on finding $N+1$ points $\underline{x}$ such that $\mathbf{T}_N(\underline{x})$ is well-conditioned. Reichel and Opfer showed that $\mathbf{T}_N(\underline{x})$ is well-conditioned when $\underline{x}$ is a set of points on a certain Bernstein ellipse [29]. Gautschi in [20, (27)] gives an explicit formula for the condition number of $\mathbf{T}_N(\underline{x})$ for any point set $\underline{x}$ in the Frobenius norm and showed that $\mathbf{T}_N(\underline{x}^{cheb})D^{-1/2}$ is the only perfectly conditioned matrix among all so-called Vandermonde-like matrices [20]. A survey of this research area can be found here [19, Sec. V].

3. How good is equally spaced least squares polynomial fitting?. We now turn our attention to solving the least squares problem in (1), where $M < N$. We are interested in the normal equations in (8) and the condition number of the $(M+1)\times(M+1)$ matrix $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$. We show that the situation is very different from in Section 2 if we take $M \leq \frac{1}{2}\sqrt{N}$. In particular, $\kappa_2(\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi}))$ is bounded with N and grows modestly with M if $M \leq \frac{1}{2}\sqrt{N}$. This means that the Chebyshev coefficients for $p_M(x)$ in (1) are not sensitive to the perturbations in $\underline{f}+\underline{\varepsilon}$ and can be computed accurately in double precision.

To bound the condition number of $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$ we can no longer use the matrix decomposition in (13) as that is not applicable when $M < N$. Instead, we first consider the normal equations for the Legendre–Vandermonde[5] matrix

$$\mathbf{P}_M(\underline{x}^{equi}) = \begin{bmatrix} P_0(x_0^{equi}) & \cdots & P_M(x_0^{equi}) \\ \vdots & \ddots & \vdots \\ P_0(x_N^{equi}) & \cdots & P_M(x_N^{equi}) \end{bmatrix} \in \mathbb{R}^{(N+1)\times(M+1)} \tag{15}$$

[5]The Legendre–Vandermonde matrix in (15) is the same as the Chebyshev–Vandermonde matrix except the Chebyshev polynomials are replaced by Legendre polynomials.

and $P_k(x)$ is the Legendre polynomial of degree k [28, Sec. 18.3]. Legendre polynomials are theoretically convenient for us because they are orthogonal with respect to the standard L^2 inner-product [28, (18.2.1) & Tab. 18.3.1], i.e.,

$$\int_{-1}^{1} P_m(x)P_n(x)dx = \begin{cases} \frac{2}{2n+1}, & m=n, \\ 0, & m \neq n, \end{cases} \qquad 0 \leq m,n \leq M. \tag{16}$$

Afterwards, in Theorem 8 we go back to consider $\kappa_2(\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi}))$.

To bound the condition number of $\mathbf{P}_M(\underline{x}^{equi})^*\mathbf{P}_M(\underline{x}^{equi})$ our key insight is to view the (m,n) entry of $\frac{2}{N}\mathbf{P}_M(\underline{x}^{equi})^*\mathbf{P}_M(\underline{x}^{equi})$ as essentially a trapezium rule approximation of the integral in (16). Since $\kappa_2(\mathbf{P}_M(\underline{x}^{equi})^*\mathbf{P}_M(\underline{x}^{equi}))$ equals $\sigma_1(\mathbf{P}_M(\underline{x}^{equi}))^2$ divided by $\sigma_{M+1}(\mathbf{P}_M(\underline{x}^{equi}))^2$, Theorem 7 focuses on bounding the squares of the maximum and minimum singular values of $\mathbf{P}_M(\underline{x}^{equi})$.

Theorem 7. *For any integers M and N satisfying $M \leq \frac{1}{2}\sqrt{N}$ we have*

$$\sigma_1\big(\mathbf{P}_M(\underline{x}^{equi})\big)^2 \leq 2N, \quad \sigma_{M+1}\big(\mathbf{P}_M(\underline{x}^{equi})\big)^2 \geq \frac{2N}{5(2M+1)}.$$

(Tighter but messy bounds can be found in (19) and (20).)

Proof. If $M=0$, then $\mathbf{P}_M(\underline{x}^{equi})$ is the $(N+1)\times 1$ vector of all ones. Thus, $\sigma_1\big(\mathbf{P}_M(\underline{x}^{equi})\big)^2 = N$ and the bounds above hold. For the remainder of this proof we assume that $M \geq 1$ and hence, $N \geq 4$.

From the orthogonality of Legendre polynomials in (16) we define

$$D_{mn} = \frac{N}{2}\int_{-1}^{1} P_m(x)P_n(x)dx = \begin{cases} \frac{N}{2n+1}, & m=n, \\ 0, & m\neq n, \end{cases} \qquad 0 \leq m,n \leq M.$$

The $(N+1)$-point trapezium rule (see (35)) provides another expression for D,

$$D = \mathbf{P}_M(\underline{x}^{equi})^*\mathbf{P}_M(\underline{x}^{equi}) - C - \frac{N}{2}E, \qquad C_{mn} = \begin{cases} 1, & m+n \text{ is even}, \\ 0, & m+n, \text{ is odd}, \end{cases} \tag{17}$$

where C is the matrix that halves the contributions at the endpoints and E is the matrix of trapezium rule errors. By the Euler–Maclaurin error formula [25, Cor. 3.3] we have, for $0 \leq m,n \leq M$,

$$E_{mn} = 2\sum_{s=1, s \text{ odd}}^{m+n-1} \frac{((P_m(1)P_n(1))^{(s)} - (P_m(-1)P_n(-1))^{(s)})2^s B_{s+1}}{N^{s+1}(s+1)!},$$

where B_s is the sth Bernoulli number and $(P_m(1)P_n(1))^{(s)}$ is the sth derivative of $P_m(x)P_n(x)$ evaluated at 1. By Markov's brother inequality $|(P_m(1)P_n(1))^{(s)}| \leq 2^s s!(m+n)^{2s}/(2s)!$ [6, p. 254] and since $|B_{s+1}| \leq 4(s+1)!(2\pi)^{-s-1}$ [28, (24.9.8)] we have

$$|E_{mn}| \leq \frac{8}{\pi N}\sum_{s=1, s \text{ odd}}^{m+n-1}\left(\frac{8}{\pi}\right)^s \frac{s!}{(2s)!}\frac{((m+n)/2)^{2s}}{N^s} \leq \frac{3(m+n)^2}{\pi N^2},$$

where in the last inequality we used $((m+n)/2)^2/N \leq M^2/N \leq 1$ and the fact that $\sum_{s=1, s \text{ odd}}^{m+n-1}(8/\pi)^s s!/(2s)! \leq 3/2$. Using $\|E\|_2 \leq \|E\|_F$, $(\sum_{m,n=0}^{M}(m+n)^4)^{1/2} \leq 9M^3/2$, and $M \leq \frac{1}{2}\sqrt{N}$, where $\|\cdot\|_F$ denotes the matrix Frobenius norm, we obtain

$$\|E\|_2 \leq \frac{27M^3}{2\pi N^2} \leq \frac{27}{16\pi\sqrt{N}}. \tag{18}$$

By Weyl's inequality on the eigenvalues of perturbed Hermitian matrices [36], we conclude that

$$\left|\lambda_k\left(\mathbf{P}_M(\underline{x}^{equi})^*\mathbf{P}_M(\underline{x}^{equi})\right) - \lambda_k(D+C)\right| \leq \tfrac{N}{2}\|E\|_2, \qquad 1 \leq k \leq M+1,$$

where $\lambda_k(A)$ denotes the kth eigenvalue of the Hermitian matrix A. By Lemma 17 we have $\lambda_1(D+C) \leq (2N+M+3)/2$ and $\lambda_{M+1}(D+C) \geq (N-M^2/2)/(2M+1)$. Since $\sigma_k(A)^2 = \lambda_k(A^*A)$ for any real matrix A, we obtain

$$\sigma_1\left(\mathbf{P}_M(\underline{x}^{equi})\right)^2 \leq \frac{2N+M+3}{2} + \frac{27\sqrt{N}}{32\pi} \tag{19}$$

and

$$\sigma_{M+1}\left(\mathbf{P}_M(\underline{x}^{equi})\right)^2 \geq \frac{N-M^2/2}{2M+1} - \frac{27\sqrt{N}}{32\pi}. \tag{20}$$

The statement follows since for $M \leq \frac{1}{2}\sqrt{N}$ and $N \geq 4$ we have $(2N+M+3)/2 + (27\sqrt{N})/(32\pi) \leq 2N$ and $(N-M^2/2)/(2M+1) - (27\sqrt{N})/(32\pi) \geq 2N/(5(2M+1))$.□

Theorem 7 shows that if $M \leq \frac{1}{2}\sqrt{N}$, then

$$\kappa_2(\mathbf{P}_M(\underline{x}^{equi})^*\mathbf{P}_M(\underline{x}^{equi})) \leq 5(2M+1).$$

This means that when $M \leq \frac{1}{2}\sqrt{N}$ we can solve for the Legendre coefficients of $p_M(x)$ in (1) via the normal equations,

$$\mathbf{P}_M(\underline{x}^{equi})^*\mathbf{P}_M(\underline{x}^{equi})\underline{c}^{leg} = \mathbf{P}_M(\underline{x}^{equi})^*\left(\underline{f} + \underline{\varepsilon}\right), \tag{21}$$

without severe ill-conditioning. Here, $\underline{c}^{leg}$ is the vector of coefficients so that

$$p_M(x) = \sum_{k=0}^{M} c_k^{leg} P_k(x).$$

Hence, the least squares problem in (1) is a practical way to construct a polynomial approximant of a function from equally spaced samples.

The bounds in Theorem 7 are essentially tight. In Figure 2 we compare the bounds in (19) and (20) to computed values of the square of maximum and minimum singular values of $\mathbf{P}_M(\underline{x}^{equi})$ when $M = \lfloor \frac{1}{2}\sqrt{N} \rfloor$. The jagged nature of the bound in Figure 2 is due to the floor function in the formula for M to ensure it is an integer. This causes jumps in the bounds at each square number.

One can also use Theorem 7 to safely compute the Chebyshev coefficients of the polynomial $p_M(x)$ in (1) too. Let S be the $(M+1)\times(M+1)$ change of basis matrix that takes Legendre coefficients to Chebyshev coefficients. The entries of S have an explicit formula given by [5, (2.18)]

$$S_{ij} = \begin{cases} \frac{1}{\pi}\Psi\left(\frac{j}{2}\right)^2, & 0 = i \leq j \leq M,\ j \text{ even}, \\ \frac{2}{\pi}\Psi\left(\frac{j-i}{2}\right)\Psi\left(\frac{j+i}{2}\right), & 0 < i \leq j \leq M,\ i+j \text{ even}, \\ 0, & \text{otherwise}, \end{cases} \tag{22}$$

where $\Psi(i) = \Gamma(i+1/2)/\Gamma(i+1)$ and $\Gamma(x)$ is the Gamma function. Theorem 7 shows that when $M \leq \frac{1}{2}\sqrt{N}$ the Legendre coefficients $\underline{c}^{leg}$ of $p_M(x)$ in (1) can be computed

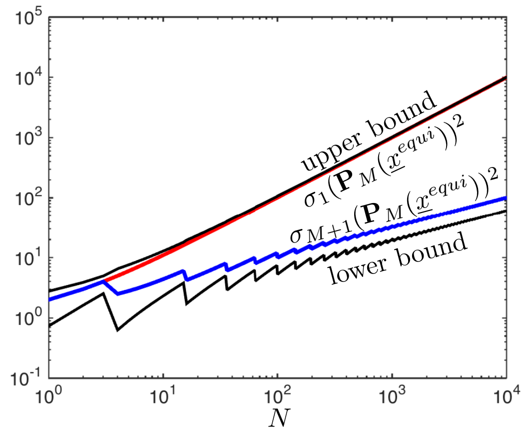

FIG. 2. *Illustration of the bounds on the squares of the maximum and minimum singular values of $\mathbf{P}_M(\underline{x}^{equi})$ as found in (19) and (20) when $M = \lfloor \frac{1}{2}\sqrt{N} \rfloor$. The statement of Theorem 7 provides simplified and slightly weaker bounds.*

accurately via the normal equations in (21). Afterwards, the Legendre coefficients, $\underline{c}^{leg}$, for $p_M(x)$ can be converted into Chebyshev coefficients, $\underline{c}^{cheb}$, for $p_M(x)$ by a matrix-vector product, i.e., $\underline{c}^{cheb} = S\underline{c}^{leg}$. For fast algorithms to compute the matrix-vector product $S\underline{c}^{leg}$, see [5, 23].

We rarely compute the Chebyshev coefficients of $p_M(x)$ via the Legendre coefficients from (21). Instead, we directly compute the Chebyshev coefficients via the normal equations in (8) because we have a fast direct algorithm (see Section 7). Here, is the bound we obtain on $\kappa_2(\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi}))$.

THEOREM 8. *For any integers M and N satisfying $M \leq \frac{1}{2}\sqrt{N}$ we have*

$$\sigma_1\big(\mathbf{T}_M(\underline{x}^{equi})\big)^2 \leq 3N, \qquad \sigma_{M+1}\big(\mathbf{T}_M(\underline{x}^{equi})\big)^2 \geq \frac{1}{25}\sigma_{M+1}\big(\mathbf{P}_M(\underline{x}^{equi})\big)^2.$$

Proof. By the trapezium rule (see (36)) we have

$$\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi}) = F + C + \tfrac{N}{2}\widetilde{E},$$

where $\widetilde{E}$ is the matrix of trapezium errors, C is given in (17), and F is given by

$$F_{mn} = \frac{N}{2}\int_{-1}^{1} T_m(x)T_n(x)dx = \frac{N}{2}\left[\frac{1}{1-(m+n)^2} + \frac{1}{1-(m-n)^2}\right]. \tag{23}$$

By the same argument as in Theorem 7 we have $\|\widetilde{E}\|_2 \leq 27/(16\pi/\sqrt{N})$, see (18). Also by Lemma 18 we have $\lambda_1(F+C) \leq (4N+M+1)/2$ and hence, using Weyl's inequality on the eigenvalues of perturbed Hermitian matrices [36] we obtain

$$\sigma_1\big(\mathbf{T}_M(\underline{x}^{equi})\big)^2 \leq \frac{4N+M+1}{2} + \frac{27\sqrt{N}}{32\pi} \leq 3N,$$

where the last inequality holds since $M \leq \frac{1}{2}\sqrt{N}$.

Next, by the definition of the matrix S in (22) we have $\mathbf{T}_M(\underline{x}^{equi})S = \mathbf{P}_M(\underline{x}^{equi})$. Hence,

$$\sigma_{M+1}\left(\mathbf{T}_M(\underline{x}^{equi})\right)^2 \geq \|S\|_2^{-2}\sigma_{M+1}\left(\mathbf{P}_M(\underline{x}^{equi})\right)^2.$$

The lower bound on $\sigma_{M+1}\left(\mathbf{T}_M(\underline{x}^{equi})\right)$ follows from Lemma 19, which proves $\|S\|_2 \leq 5$. ∎

Theorem 8 bounds the condition number of $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$. If $M \leq \frac{1}{2}\sqrt{N}$, then

$$\kappa_2(\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})) \leq \frac{375}{2}(2M+1). \tag{24}$$

Therefore, the Chebyshev coefficients, $\underline{c}^{cheb}$, of $p_M(x)$ in (1) can be computed accurately via the normal equations in (8).

The lower bound on the minimum singular value of $\mathbf{T}_M(\underline{x}^{equi})$ shows that the solution vector $\underline{c}^{cheb}$ is not sensitive to small perturbations in the function samples and is the key result for sections 5 and 6.

The $M \leq \frac{1}{2}\sqrt{N}$ assumption in Theorem 8 can in practice be slightly violated without consequence, for example, $M \leq 2\sqrt{N}$ gives the same qualitative behavior. We can even improve the restriction in Theorem 8 to $M \leq 0.95\sqrt{N}$ and use the same argument to show that $\kappa_2(\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi}))$ grows linearly with M. Unfortunately, the derived bounds are so awkward to write down that they are not worthwhile in a paper of this nature. We certainly do not pretend that the constants in Theorem 7 and Theorem 8 are tight, though we are pleased that the bounds are explicit.

During the final stages of writing this paper we were made aware of [4, Thm. 5.1], which as a special case also gives a similar, but non-explicit, bound as in Theorem 8. Since we are using very specific techniques, the bounds in Theorem 8 have explicit constants.

4. Approximation power of least squares polynomial fitting. In this section, we derive results to understand how well p_M approximates f on $[-1,1]$ under the assumption that $\varepsilon = 0$, i.e., the function samples are not perturbed.

The following theorem allows for any $M \leq N$, though afterwards we restrict $M \leq \frac{1}{2}\sqrt{N}$ so that $\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))$ can be bounded from below using Theorem 8.

THEOREM 9. *Let M and N be integers satisfying $M \leq N$ and $\varepsilon = 0$. Let f be an analytic function with Bernstein parameter $\rho > 1$ and $\underline{c}^{cheb}$ be the vector of Chebyshev coefficients of the degree M polynomial p_M in (1). Then, we have*

$$|c_k^{cheb}| \leq 2Q\left[\rho^{-k} + \frac{(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}\frac{\rho^{-M}}{\rho-1}\right], \qquad 0 \leq k \leq M,$$

and

$$\|f - p_M\|_\infty \leq 2Q\left[1 + \frac{(M+1)(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}\right]\frac{\rho^{-M}}{\rho-1},$$

where $\|f - p_M\|_\infty = \sup_{x\in[-1,1]}|f(x) - p_M(x)|$.

Proof. Let f_M be the polynomial of degree M constructed by truncating the Chebyshev expansion for f after $M+1$ terms, see Proposition 4. Then,

$$f(\underline{x}^{equi}) = f_M(\underline{x}^{equi}) + f(\underline{x}^{equi}) - f_M(\underline{x}^{equi}) = \mathbf{T}_M(\underline{x}^{equi})\underline{a}_M + (f - f_M)(\underline{x}^{equi}),$$

where $\underline{a}_M$ is the vector of the first $M+1$ Chebyshev coefficients for f. The vector $\underline{c}^{cheb}$ satisfies the normal equations, $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})\underline{c}^{cheb} = \mathbf{T}_M(\underline{x}^{equi})^* f(\underline{x}^{equi})$, and since $f_M(\underline{x}^{equi}) = \mathbf{T}_M(\underline{x}^{equi})\underline{a}_M$ we have

$$\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})(\underline{c}^{cheb} - \underline{a}_M) = \mathbf{T}_M(\underline{x}^{equi})^*(f - f_M)(\underline{x}^{equi}).$$

Noting that $\|(A^*A)^{-1}A^*\|_2 = 1/\sigma_{\min}(A)$ for any matrix A, we have the following bound:

(25)

$$\begin{aligned}\|\underline{c}^{cheb} - \underline{a}_M\|_\infty &\leq \|(\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi}))^{-1}\mathbf{T}_M(\underline{x}^{equi})^*\|_\infty \|(f - f_M)(\underline{x}^{equi})\|_\infty \\ &\leq 2Q\frac{(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}\frac{\rho^{-M}}{\rho - 1},\end{aligned}$$

where in the last inequality we used $\|(f - f_M)(\underline{x}^{equi})\|_\infty \leq 2Q\rho^{-M}/(\rho - 1)$ (see Proposition 4) and $\|A\|_\infty \leq \sqrt{N+1}\|A\|_2$ for matrices of size $(M+1)\times(N+1)$. The bound on $|c_k^{cheb}|$ follows since $|c_k^{cheb}| \leq |a_k| + \|\underline{c}^{cheb} - \underline{a}_M\|_\infty$ and $|a_k| \leq 2Q\rho^{-k}$ for $k \geq 0$ (see Proposition 4).

For a bound on $\|f - p_M\|_\infty$, note that $T_k(x) \leq 1$ for $k \geq 0$ and $x \in [-1, 1]$. Hence,

$$\|f - p_M\|_\infty \leq (M+1)\|\underline{c}^{cheb} - \underline{a}_M\|_\infty + \sum_{k=M+1}^{\infty}|a_k| \leq 2Q\left[1 + \frac{(M+1)(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}\right]\frac{\rho^{-M}}{\rho - 1},$$

where we again used $|a_k| \leq 2Q\rho^{-k}$ for $k \geq 0$. ◻

When $M \leq \frac{1}{2}\sqrt{N}$ we can use Theorem 9 together with the lower bound on $\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))$ from Theorem 8 to conclude that

$$\|f - p_M\|_\infty \leq 2Q\left[1 + 10\sqrt{5}(M+1)^{3/2}\right]\frac{\rho^{-M}}{\rho - 1}. \tag{26}$$

Thus, with respect to M, the least squares polynomial fit p_M converges geometrically to f with order ρ. Along with the bound on the condition number of the normal equations in (24), it confirms that least squares polynomial approximation is a practical tool for approximating analytic functions given equally spaced samples.

It is common to refer to (26) as a subexponential convergence rate because one needs to take $\mathcal{O}(N)$ equally spaced samples to realize an approximation error of $\mathcal{O}(\rho^{-\sqrt{N}})$. We now use the noisy bounds to consider the case when the function samples are perturbed, i.e., $\varepsilon > 0$.

5. Least squares polynomial fitting is robust to noisy samples. Polynomial interpolation at equally spaced points is sensitive to noisy function samples samples, and this is a considerable drawback. In contrast, when there is sufficient oversampling, i.e., $M \leq \frac{1}{2}\sqrt{N}$, least squares polynomial fits are robust to perturbed function samples. In this section we consider two cases: The vector of function samples $f(\underline{x}^{equi})$ is perturbed by either a vector of independent Gaussian random variables with mean 0 and known variance s^2 or a vector of deterministic errors given by $\underline{\varepsilon}$ with known maximum amplitude $\|\underline{\varepsilon}\|_\infty$.

5.1. Least squares polynomial fitting with Gaussian noise. First suppose that the samples are given by $f(\underline{x}^{equi}) + \underline{\varepsilon}$, where $\underline{\varepsilon} = (\varepsilon_0, \ldots, \varepsilon_N)^T$ is a vector with entries that are independent Gaussian random variables with mean 0 and variation

s^2, i.e., $\varepsilon_k \sim \mathcal{N}(0, s^2)$ for $0 \leq k \leq N$. We refer to the standard deviation of the noise, s, as the *noise level*.

Thus, we seek the solution to the perturbed normal equations,

$$\mathbf{T}_M(\underline{x}^{equi})^* \mathbf{T}_M(\underline{x}^{equi}) \underline{c}^{cheb} = \mathbf{T}_M(\underline{x}^{equi})^* \left(\underline{f} + \underline{\varepsilon} \right). \tag{27}$$

The vector of Chebyshev coefficients $\underline{c}^{cheb}$ for the least squares fit $p_M(x)$ are now a vector of random variables. It is easy to see that the expectation of the vector $\underline{c}^{cheb}$ is given by

$$\mathbb{E}\left[\underline{c}^{cheb}\right] = (\mathbf{T}_M(\underline{x}^{equi})^* \mathbf{T}_M(\underline{x}^{equi}))^{-1} \mathbf{T}_M(\underline{x}^{equi})^* \underline{f},$$

which verifies that the expectation of the coefficients is the same as in the noiseless case. To get a bound on the expectation of the approximation error $\|f - p_M\|_\infty$ we need to bound the variance of $\underline{c}^{cheb}$. Here, is one such bound that we state for any $M \leq N$, though afterwards we restrict ourselves to $M \leq \frac{1}{2}\sqrt{N}$.

LEMMA 10. *Let M and N be integers satisfying $M \leq N$ and let $\underline{\varepsilon} \in \mathbb{R}^{(N+1)\times 1}$ be a vector with entries that are realizations from independent and identically distributed Gaussian random variables with mean 0 and variance s^2. Then, for the vector $\underline{c}^{cheb}$ satisfying (27) we have*

$$\mathbb{E}\left[\left\|\underline{c}^{cheb} - \mathbb{E}\left[\underline{c}^{cheb}\right]\right\|_2^2\right] \leq \frac{(M+1)s^2}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))^2},$$

where $\mathbb{E}[X]$ denotes the expectation of the random variable X.

Proof. Let $A = \mathbf{T}_M(\underline{x}^{equi})$ and note that

$$\mathbb{E}\left[\left\|\underline{c}^{cheb} - \mathbb{E}\left[\underline{c}^{cheb}\right]\right\|_2^2\right] = \mathbb{E}\left[\left\|(A^*A)^{-1}A^*\underline{\varepsilon}\right\|_2^2\right].$$

Let $P = A(A^*A)^{-1}A^* \in \mathbb{C}^{(N+1)\times(N+1)}$ be the orthogonal projection of $\mathbb{C}^{N+1}$ onto the range of A. Since $(A^*A)^{-1}A^* = (A^*A)^{-1}A^*P$, $\|(A^*A)^{-1}A^*\|_2 = \sigma_{M+1}(A)^{-1}$, and[6] $\mathbb{E}[\|P\underline{\varepsilon}\|_2^2] \leq (M+1)s^2$, we have

$$\mathbb{E}\left[\|(A^*A)^{-1}A^*\underline{\varepsilon}\|_2^2\right] = \mathbb{E}\left[\|(A^*A)^{-1}A^*P\underline{\varepsilon}\|_2^2\right] \leq \|(A^*A)^{-1}A^*\|_2^2\, \mathbb{E}\left[\|P\underline{\varepsilon}\|_2^2\right] \leq \frac{(M+1)s^2}{\sigma_{M+1}(A)^2},$$

as required. ∎

Lemma 10 shows that the sum of the variances of the entries of $\underline{c}^{cheb}$ is comparable to the sum of the variances of $\underline{\varepsilon}$, provided that $\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))$ is not too small. Thus, if $\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))$ is sufficiently large, then we expect $p_M(x)$ to be stable under small perturbations of the function samples. We show this by bounding the expected maximum uniform error between f and p_M.

COROLLARY 11. *Suppose the assumptions of Lemma 10 hold, f is an analytic function with Bernstein parameter $\rho > 1$, and p_M is the least squares polynomial fit of degree M in (1). Then,*

$$\mathbb{E}\left[\|f - p_M\|_\infty\right] \leq \frac{(M+1)^{3/2}s}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))} + 2Q\left[1 + \frac{(M+1)(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}\right]\frac{\rho^{-M}}{\rho - 1}. \tag{28}$$

---

[6] Let $A = QR$ be the reduced QR factorization of A, where $Q = \left[\underline{q}_0 \mid \cdots \mid \underline{q}_M\right]$. Then, $\|P\underline{\varepsilon}\|_2^2 = \underline{\varepsilon}^*P^*P\underline{\varepsilon} = \underline{\varepsilon}^*QQ^*\underline{\varepsilon} = \sum_{k=0}^M |\underline{q}_k^*\underline{\varepsilon}|^2$. Since $\mathbb{E}[|\underline{q}_k^*\underline{\varepsilon}|^2] = s^2$ we have $\mathbb{E}[\|P\underline{\varepsilon}\|_2^2] \leq (M+1)s^2$.

Moreover, when $M \leq \frac{1}{2}\sqrt{N}$ *we have*

$$\mathbb{E}\left[\|f - p_M\|_\infty\right] \leq \frac{5\sqrt{5}(M+1)^2 s}{N^{1/2}} + 2Q\left[1 + 10\sqrt{5}(M+1)^{3/2}\right]\frac{\rho^{-M}}{\rho - 1}, \tag{29}$$

where $\|f - p_M\|_\infty = \sup_{x\in[-1,1]} |f(x) - p_M(x)|$.

Proof. The same reasoning as in Theorem 9, but with an extra term allowing for the noisy samples, gives the bound

$$\begin{aligned}\mathbb{E}\left[|f(x) - p_M(x)|\right] \leq 2Q\left[1 + \frac{(M+1)(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}\right]\frac{\rho^{-M}}{\rho-1} \\ + \mathbb{E}\left[\left|\sum_{k=0}^{M}(\underline{c}^{cheb} - \mathbb{E}[\underline{c}^{cheb}])_k T_k(x)\right|\right].\end{aligned}$$

Since $|T_k(x)| \leq 1$ and $\mathbb{E}[X]^2 \leq \mathbb{E}[X^2]$, this extra term can be bounded as follows:

$$\begin{aligned}\mathbb{E}\left[\left|\sum_{k=0}^{M}(\underline{c}^{cheb} - \mathbb{E}[\underline{c}^{cheb}])_k T_k(x)\right|\right]^2 &\leq \mathbb{E}\left[\left\|\underline{c}^{cheb} - \mathbb{E}[\underline{c}^{cheb}]\right\|_1^2\right] \\ &\leq (M+1)^2\mathbb{E}\left[\left\|\underline{c}^{cheb} - \mathbb{E}[\underline{c}^{cheb}]\right\|_2^2\right],\end{aligned}$$

where Lemma 10 can now be employed. For the second statement, substitute the bound derived in (26) into (28). ◻

Therefore, when $M \leq \frac{1}{2}\sqrt{N}$ the least squares polynomial fit $p_M(x)$ in (1) is robust to noisy equally spaced samples of f. On closer inspection of the bound in (29), we find that $\|f - p_M\|_\infty$ decays geometrically with order ρ, until it plateaus at roughly $5\sqrt{5}(M+1)^2/\sqrt{N}s$. Since $M \approx \frac{1}{2}\sqrt{N}$ the plateau is proportional to the noise level s, even as $N \to \infty$.

One interesting regime is to keep M fixed and to increase the number of samples $N+1$. We see that $\|f - p_M\|_\infty$ is about $\mathcal{O}(s/\sqrt{N})$ in size. Intuitively, this makes sense because one could imagine averaging nearby samples onto a coarser equally spaced grid and using those averaged samples instead. Since the variance of an average of independent random variables scales like the reciprocal of the number in the average, we expect $\|f - p_M\|_\infty$ to plateau at about $\mathcal{O}(s/\sqrt{N})$. Figure 3 shows a related phenomenon on the plateau of the Chebyshev coefficients of the least squares polynomial fit $p_M(x)$ to $f(x) = 1/(1 + 25(x - 1/100)^2)$ on $[-1, 1]$. If the number of samples is increased by a factor of 100, then the plateau of the Chebyshev coefficients drops by a factor of 10, which confirms the $s/\sqrt{N}$ behavior.

5.2. Least squares polynomial fitting with deterministic perturbations. Now suppose that $f(\underline{x}^{equi})$ is polluted with deterministic error such as $f(\underline{x}^{equi}) + \underline{\varepsilon}$, where $\underline{\varepsilon} = (\varepsilon_0, \ldots, \varepsilon_N)^T$ is a vector such that $\|\underline{\varepsilon}\|_\infty = \varepsilon < \infty$. We wish to solve

$$\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})\underline{c}^{cheb} = \mathbf{T}_M(\underline{x}^{equi})^*\left(\underline{f} + \underline{\varepsilon}\right)$$

and understand the quality of the resulting least squares polynomial fit p_M. This is relatively easy to do given the proof of Theorem 9 so we state it as a corollary.

Corollary 12. *Suppose that the assumptions in Theorem 9 are satisfied, and that the values of* $\underline{f}$ *are perturbed by a vector* $\underline{\varepsilon}$*, where* $\|\underline{\varepsilon}\|_\infty = \varepsilon < \infty$*. Then,*

$$\|f - p_M\|_\infty \leq 2Q\left[1 + \frac{(M+1)(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}\right]\frac{\rho^{-M}}{\rho-1} + \frac{(M+1)(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}\varepsilon.$$

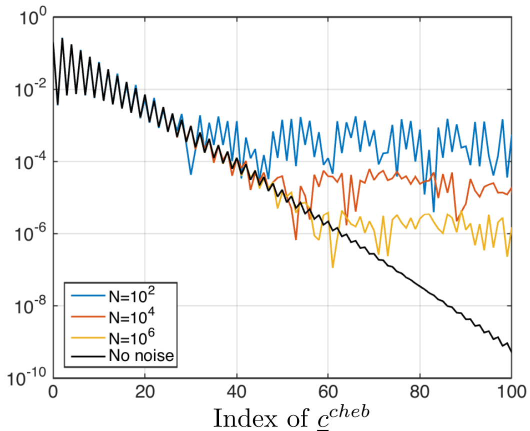

FIG. 3. *The Chebyshev coefficients of $p_M(x)$ in (1) when $M = 100$, $f(x) = 1/(1+25(x-1/100)^2)$, and the function samples are perturbed by white noise with a standard deviation of 10^{-3}. The shift of $1/100$ in the definition of f is to prevent the function from being even, simplifying the plot. When the number of equally spaced samples is increased by a factor of 100, the plateau in the tail of the coefficients drops by a factor of 10 (see Corollary 11).*

Proof. The same proof as Theorem 9 except with an additional term that is easy to bound due to the vector $\underline{\varepsilon}$. ∎

By taking $M \leq \frac{1}{2}\sqrt{N}$ and noting that $\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))^2 \geq 2N/(125(2M+1))$ we see that p_M does not converge to f as $N \to \infty$ with deterministic error, though it plateaus at around $\mathcal{O}(\varepsilon)$. If M is fixed and $N \to \infty$, then Corollary 12 shows that $\|f - p_M\|_\infty$ remains bounded. This is to be expected because in this situation one cannot average a dense set of function samples onto a coarse grid and reduce the uncertainty in the sampled values.

6. Stable extrapolation with least squares polynomial fits. Without perturbed function samples a least squares polynomial fit from equally spaced samples can be used to extrapolate outside of $[-1,1]$, by a distance that depends on the analyticity of the sampled function. However, in practice polynomial extrapolation is sensitive to perturbed samples or roundoff errors in floating point arithmetic.

In sections 6.2 and 6.3 we go further and show that there are two interesting regimes: (1) if the noise is modeled by independent Gaussian random variables and there is exponential oversampling, i.e., $N = e^{aM}$, then one can stably extrapolate to $x \in I_\rho = [1, (\rho + 1/\rho)/2)$, and (2) if the noise in the function samples is deterministic, then there is a degree M^* that (nearly) minimizes $\sup_{x\in I_\rho} |f(x) - p_M(x)|$. If $M^* < N/2$, then the minimum extrapolation error is a x-dependent fractional power of ε.

6.1. Extrapolation without noise. Without noise in the function samples, it turns out that one can extrapolate by any x satisfying $1 \leq x < (\rho + \rho^{-1})/2$. In fact, one cannot expect to extrapolation any further than $(\rho + \rho^{-1})/2$ with a polynomial approximant because f is only assumed to be bounded and analytic in an ellipse that intercepts the x-axis at $(\rho + \rho^{-1})/2$.

THEOREM 13. *Suppose that the assumptions in Theorem 9 hold. Then, for any*

$1 < x < (\rho + \rho^{-1})/2$ *we have*

$$|f(x) - p_M(x)| \leq 2Q \left[\frac{(N+1)^{1/2}(M+1)}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))(\rho - 1)} + \frac{r}{1-r} \right] r^M,$$

where $r = (x + \sqrt{x^2 - 1})/\rho < 1$*. In other words, it is possible to use* $p_M(x)$ *to extrapolate outside of* $[-1, 1]$ *by a distance determined by the analyticity of* f*.*

Proof. Since $|T_k(x)| \leq (x + \sqrt{x^2 - 1})^k$ for $x > 1$ we have, by Theorem 9 and Proposition 4,

$$\begin{aligned}
|f(x) - p_M(x)| &\leq \sum_{k=0}^{M} |a_k - c_k^{cheb}||T_k(x)| + \sum_{k=M+1}^{\infty} |a_k||T_k(x)| \\
&\leq \|\underline{a}_M - \underline{c}^{cheb}\|_\infty \sum_{k=0}^{M} |T_k(x)| + 2Q \sum_{k=M+1}^{\infty} \rho^{-k}|T_k(x)| \\
&\leq 2Q \left[\frac{(N+1)^{1/2}}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))} \frac{\rho^{-M}}{\rho - 1} \sum_{k=0}^{M} \rho^k r^k + r^{M+1} \sum_{k=0}^{\infty} r^k \right],
\end{aligned}$$

where the last inequality used (25) and $r = (x + \sqrt{x^2 - 1})/\rho$. Since $1 < x < (\rho + \rho^{-1})/2$ we have $r < 1$ and by the sum of a geometric series we conclude that

$$|f(x) - p_M(x)| \leq 2Q \left[\frac{(N+1)^{1/2}(M+1)}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))(\rho - 1)} + \frac{r}{1-r} \right] r^M,$$

where we used the inequality $\sum_{k=0}^{M} \rho^k r^k \leq (M+1)\rho^M r^M$. ∎

Figure 4 verifies Theorem 13 for $f(x) = 1/(1 + x^2)$ and $g(x) = 1/(1 + 2x^2)$. Let p and q be the least squares polynomial fits to f and g of degree M constructed by $N + 1$ equally spaced samples with $M \leq \frac{1}{2}\sqrt{N}$. Since $\rho = 2.42$ is the Bernstein parameter for f and $\rho = 4.24$ for g, Theorem 13 predicts that the least squares error $|f(x) - p_M(x)|$ and $|g(x) - q(x)|$ geometrically decays to zero as $M \to \infty$ for $1 < x < \sqrt{2}$ and $1 < x < 1.23$, respectively. This is observed in Figure 4.

6.2. Extrapolation with Gaussian noise. In the presence of noise in the function samples one must be a little more careful. Suppose that the functions samples, $f(\underline{x}^{equi})$, are perturbed by noise, $f(\underline{x}^{equi}) + \underline{\varepsilon}$, so that each entry of $\underline{\varepsilon}$ is modeled by a Gaussian random variable with mean 0 and variable s^2. Then, the expected extrapolation error can be bounded as follows:

Corollary 14. *Suppose that the assumptions in Corollary 11 hold. Then, for any* $1 \leq x < (\rho + \rho^{-1})/2$ *we have*

$$\mathbb{E}\left[|f(x) - p_M(x)|\right] \leq 2Q \left[\frac{(N+1)^{1/2}(M+1)}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))(\rho - 1)} + \frac{r}{1-r} \right] r^M + \frac{(M+1)^{3/2} s}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))} (\rho r)^M,$$

where $r = (x + \sqrt{x^2 - 1})/\rho$*.*

Proof. Essentially the same proof as Theorem 13 with an additional term that is bounded using Lemma 10. ∎

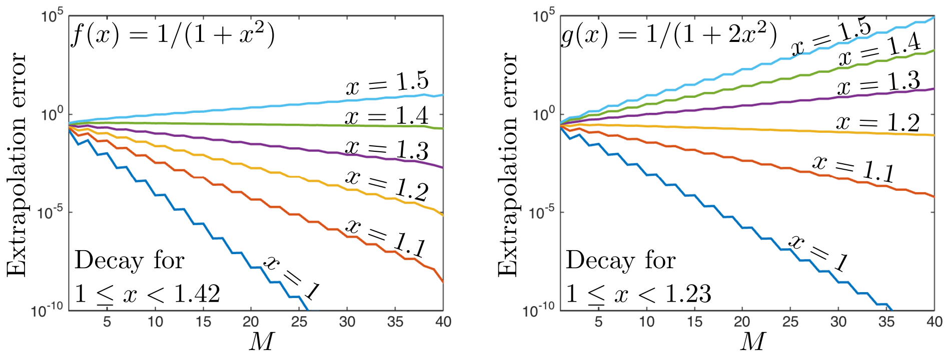

FIG. 4. *Least squares extrapolation error. Left: The error* $|f(x) - p_M(x)|$ *at* $x = 1, 1.1, 1.2, 1.3, 1.4, 1.5$, *where* $f(x) = 1/(1+x^2)$, p_M *is the least squares polynomial fit of degree* M, *and* $1 \leq M \leq 40$. *For any* $1 < x < \sqrt{2}$ *the extrapolation error* $|f(x) - p_M(x)|$ *converges geometrically with order* $r = (x + \sqrt{x^2-1})/\rho$ *to zero as* $M \to \infty$ *(see Theorem 13). Right: The same as the left figure for* $g(x) = 1/(1+2x^2)$. *For any* $1 < x < 1.23$ *the extrapolation error* $|g(x) - p_M(x)|$ *converges geometrically to zero as* $M \to \infty$, *where* p_M *is the least squares polynomial fit to* g *of degree* M.

This shows that extrapolation with noise is unstable since $\rho r > 1$ and hence, $(\rho r)^M$ grows exponentially with M. A closer look reveals a more interesting phenomenon though. When $M \leq \frac{1}{2}\sqrt{N}$, using Corollary 14, Theorem 8, and forgetting quantities that grow like a polynomial in M, we have

$$\mathbb{E}\left[|f(x) - p_M(x)|\right] \lesssim \frac{2Qr^{M+1}}{1-r}, \qquad 1 \leq x < (\rho + \rho^{-1})/2 + \frac{s(\rho r)^M}{\sqrt{N}},$$

where $r = (x + \sqrt{x^2-1})/\rho < 1$. Therefore, if the function is exponentially oversampled, i.e., $N \geq e^{aM}$ for some constant a, then

$$\mathbb{E}\left[|f(x) - p_M(x)|\right] \lesssim \frac{2Qr^{M+1}}{1-r} + sN^{\frac{1}{a}\log(\rho r) - 1/2},$$

and provided that $a > 2\log(\rho r)$ the expected extrapolation error decays to 0 as $M \to \infty$. This regime may not be as practical as one might hope because exponential oversampling is quite prohibitive; however, it reveals that polynomial extrapolation can not only be stable, but also arbitrarily accurate, with function samples perturbed by Gaussian noise.

6.3. Extrapolation with deterministic perturbations. A quite different situation occurs when the function samples are perturbed deterministically. That is, we obtain function samples of the form $f(\underline{x}^{equi}) + \underline{\varepsilon}$ with $\|\underline{\varepsilon}\|_\infty < \infty = \varepsilon < \infty$. Here, is the bound that one obtains on the extrapolation error.

COROLLARY 15. *Suppose that the assumptions in Corollary 12 hold. Then, for any fixed* $1 \leq x < (\rho + \rho^{-1})/2$ *we have*

$$|f(x) - p_M(x)| \leq 2Q\left[\frac{(N+1)^{1/2}(M+1)}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))(\rho - 1)} + \frac{r}{1-r}\right] r^M + \frac{(M+1)(N+1)^{1/2}\varepsilon}{\sigma_{M+1}(\mathbf{T}_M(\underline{x}^{equi}))}(\rho r)^M, \tag{30}$$

where $r = (x + \sqrt{x^2-1})/\rho$.

Proof. Essentially the same proof as Theorem 13 with an additional term depending on ε that is relatively simple to bound. $\square$

Since $\rho r > 1$, the upper bound in (30) does not decay to zero as $M \to \infty$. However, there is again a more interesting phenomenon here to investigate. Given an $1 \leq x < (\rho + \rho^{-1})/2$ and a perturbation level ε, we can select an integer M that (nearly) minimizes the bound in (30). Under the assumption that $M \leq \frac{1}{2}\sqrt{N}$, using Theorem 8, and by ignoring quantities that grow like a polynomial in M (and otherwise depend on ρ), we have

$$|f(x) - p_M(x)| \lesssim \frac{Qr}{1-r} r^M + (\rho r)^M \varepsilon. \tag{31}$$

We now turn to the proof of Theorem 2. We wish to find an integer $\widetilde{M}$ that approximately balances the orders of magnitude of the two terms in (31). A simple choice is

$$\widetilde{M} = \lfloor \log(Q/\varepsilon)/\log\rho \rfloor. \tag{32}$$

In this case, we get

$$|f(x) - p_{\widetilde{M}}(x)| \lesssim \frac{Q}{1-r} \left(\frac{\|\varepsilon\|_\infty}{Q}\right)^{-\log r/\log\rho}. \tag{33}$$

Notice that the integer rounding that occurs in (32) only contributes at most a factor ρ to the bound in (33) and this is absorbed in the constant. We are now ready to prove Theorem 2.

In the oversampled case, i.e., $\widetilde{M} < \frac{1}{2}\sqrt{N}$, we can let $M^* = \widetilde{M}$, and the bound in (33) is the desired result from Theorem 2.

In the undersampled case, i.e., $\widetilde{M} \geq \frac{1}{2}\sqrt{N}$, the value of $\widetilde{M}$ is too large to be admissible, so we let $M^* = \frac{1}{2}\sqrt{N}$ instead. In this case, the term $(Qr/(1-r))r^M$ dominates in equation (31), and we get

$$|f(x) - p_M(x)| \lesssim \frac{Q}{1-r} r^{\frac{1}{2}\sqrt{N}}. \tag{34}$$

This concludes the proof of Theorem 2.

6.4. Minimax rate for extrapolation with deterministic perturbations. One may wonder if it is possible to construct a more accurate extrapolant from perturbed equally spaced samples with piecewise polynomials, rational functions, or some other procedure. Here, we turn our attention to the proof of Proposition 3, which shows that this is not possible. We achieve this by constructing an analytic function $g(x)$ such that $\sup_{x\in[-1,1]} |g(x)| \leq \varepsilon$ and grows as fast as possible for $x > 1$. Any extrapolation procedure cannot distinguish between $g(x)$ and the zero function (because function values can be perturbed by ε) and therefore, no extrapolation procedure can deliver an accuracy better than $|g(x)|/2$ at $x \in I_\rho$, for both g and the zero function simultaneously.

Consider the function defined by

$$g(x) = \frac{\rho - 1}{\rho} \sum_{n \geq K} \rho^{-n} T_n(x), \qquad K = \lfloor \log(1/\varepsilon)/\log\rho \rfloor.$$

For $x \in [-1, 1]$, it is simple to bound $g(x)$ as follows:

$$|g(x)| \leq \frac{\rho - 1}{\rho} \sum_{n \geq K} \rho^{-n} = \rho^{-K-1} \leq \varepsilon.$$

To formulate a lower bound on $|g(x)|$ for $x \geq 1$, it is helpful to make use of the "partial generating function" given by

$$\sum_{n \geq K} \rho^{-n} T_n(x) = \frac{\rho^{-K-1} T_{K+1}(x) - \rho^{-K-2} T_K(x)}{1 - 2\rho^{-1} x + \rho^{-2}}, \qquad K \geq 1,$$

which can easily be proved by induction on K. The denominator can also be written as $1 - 2\rho^{-1}x + \rho^{-2} = 2\rho^{-1}(\frac{1}{2}(\rho + \rho^{-1}) - x)$, which readily shows that $f \in B_{\rho'}(Q')$ for every $\rho' < \rho$, and for some $Q' > 0$. We can now let $\rho r = x + \sqrt{x^2 - 1}$, and use the formula $T_n(x) = ((\rho r)^n + (\rho r)^{-n})/2$ to obtain

$$\begin{aligned} 2\frac{\rho^{K+2}}{\rho - 1}(1 - 2\rho^{-1}x + \rho^{-2}) g(x) &= (\rho r)^{K+1} + (\rho r)^{-(K+1)} - \rho^{-1}(\rho r)^K - \rho^{-1}(\rho r)^{-K} \\ &= (\rho r - \rho^{-1})(\rho r)^K + ((\rho r)^{-1} - \rho^{-1})(\rho r)^{-K} \\ &\geq (1 - \rho^{-1})(\rho r)^K, \end{aligned}$$

where in the last inequality we used $1 \leq \rho r \leq \rho$. Next, it is easy to see that

$$1 - 2\rho^{-1}x + \rho^{-2} = (1 - \rho^{-1}\rho_+)(1 - \rho^{-1}\rho_-),$$

where $\rho_\pm = x \pm \sqrt{x^2 - 1}$. We have $\rho^{-1}\rho_+ = r$, while $0 \leq \rho^{-1}\rho_- \leq \rho^{-1}$, so

$$1 - 2\rho^{-1}x + \rho^{-2} \leq 1 - r.$$

Therefore, we conclude that

$$g(x) \geq \frac{\rho^{-2}(1 - \rho^{-1})(\rho - 1)}{2} \frac{r^K}{1 - r} \equiv c_\rho \frac{r^K}{1 - r}, \qquad 1 \leq x < \frac{\rho + \rho^{-1}}{2},$$

where c_ρ is a constant that only depends on ρ. By recalling that the value of K is $\lfloor \log(1/\varepsilon)/\log \rho \rfloor$, we obtain

$$g(x) \geq c_\rho \frac{1}{1 - r} \varepsilon^{-\log r/\log \rho}.$$

This completes the proof of Proposition 3.

7. A faster algorithm for equally spaced least squares polynomial fitting. While conducting numerical experiments for this paper, we derived a faster direct algorithm for constructing the normal equations. We describe this algorithm now.

When $M < N$, the least squares problem in (1) is solved by the normal equations in (8), which is an $(M+1) \times (M+1)$ linear system for the Chebyshev coefficients of $p_M(x)$. Since $\mathbf{T}_M(\underline{x}^{equi})$ is an $(N+1) \times (M+1)$ matrix it naively costs $\mathcal{O}(M^2 N)$ operations to compute the matrix-matrix product $\mathbf{T}_M(\underline{x}^{equi})^* \mathbf{T}_M(\underline{x}^{equi})$, $\mathcal{O}(MN)$ operations to compute the matrix-vector $\mathbf{T}_M(\underline{x}^{equi})^* \underline{f}$, and $\mathcal{O}(M^3)$ operations to solve the resulting linear system. In this section, we show how the matrix-matrix product $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$ can be computed in just $\mathcal{O}(M^3)$ operations. When $M = \lfloor \frac{1}{2}\sqrt{N} \rfloor$ this is a computational saving as it reduces $\mathcal{O}(N^2)$ operations to construct and solve the normal equations to $\mathcal{O}(N^{3/2})$ operations.

This is a direct algorithm for constructing and solving the normal equations. Alternatively, one may use an iterative method such as the conjugate gradient method on the normal equations, where the nonuniform FFT is employed to apply the matrix $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$ to a vector in $\mathcal{O}(N \log N)$ operations. While each iteration is fast, the condition number of $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$ is $\mathcal{O}(M)$ (see 24) so one expects the conjugate gradient method to require about $\mathcal{O}(M^{1/2})$ iterations. Hence, the algorithmic complexity of the iteration approach is $\mathcal{O}(M^{1/2}N \log N)$ operations. We prefer the direct approach because the cost of constructing the normal equations is independent of N.

Our key observation is that the (m, n) entry of $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$ given by $\sum_{k=0}^{N} T_m(x_k^{equi})T_n(x_k^{equi})$, which can be thought of as a trapezium rule approximation of an integral. To see this recall that for a continuous function $h(x)$ the trapezium rule approximation to its integral is

$$\int_{-1}^{1} h(x)dx \approx \frac{1}{N}\left(h(x_0^{equi}) + 2h(x_1^{equi}) + \cdots + 2h(x_{N-1}^{equi}) + h(x_N^{equi})\right) \tag{35}$$

and hence, we have for $0 \le m, n \le M$

$$\int_{-1}^{1} T_m(x)T_n(x)dx = \frac{2}{N}\sum_{k=0}^{N} T_m(x_k^{equi})T_n(x_k^{equi}) - \frac{1}{N}(1 + (-1)^{m+n}) - \widetilde{E}_{mn}, \tag{36}$$

where $\widetilde{E}_{mn}$ is the error in the trapezium rule approximation. After rearranging, calculating the integral in (36) analytically, and noting that $\sum_{k=0}^{N} T_m(x_k^{equi})T_n(x_k^{equi}) = 0$ if $m + n$ is odd, we conclude that

$$\sum_{k=0}^{N} T_m(x_k^{equi})T_n(x_k^{equi}) = \begin{cases} \frac{N}{2(1-(m+n)^2)} + \frac{N}{2(1-(m-n)^2)} + 1 + \frac{N}{2}\widetilde{E}_{mn}, & m + n \text{ is even,} \\ 0, & \text{otherwise.} \end{cases} \tag{37}$$

The sum on the lefthand side of (37), which is used when naively computing the (m, n) entry of $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$, costs $\mathcal{O}(N)$ operations to evaluate. While the righthand side requires $\mathcal{O}(M)$ operations because of the Euler–Maclaurin error formula for $\widetilde{E}_{mn}$ [25, Cor. 3.3]. That is,

$$\widetilde{E}_{mn} = 2\sum_{s=1, s \text{ odd}}^{m+n-1} \frac{((T_m(1)T_n(1))^{(s)} - (T_m(-1)T_n(-1))^{(s)})2^s B_{s+1}}{N^{s+1}(s+1)!},$$

where B_s is the sth Bernoulli number and $(T_m(1)T_n(1))^{(s)}$ is the sth derivative of $T_m(x)T_n(x)$ evaluated at 1. By calculating $(T_m(\pm 1)T_n(\pm 1))^{(s)}$ analytically and rearranging we have

$$\widetilde{E}_{mn} = \frac{2}{N}\sum_{s=1, s \text{ odd}}^{m+n-1}\left[\prod_{j=0}^{s-1}\frac{(m-n)^2 - j^2}{N(j+1/2)} + \prod_{j=0}^{s-1}\frac{(m+n)^2 - j^2}{N(j+1/2)}\right]\frac{B_{s+1}}{(s+1)!}. \tag{38}$$

Here, the summand contains two products. The first product depends on $m - n$ and the other on $m + n$, in a Toeplitz-plus-Hankel structure. For $0 \le m, n \le M$ there are

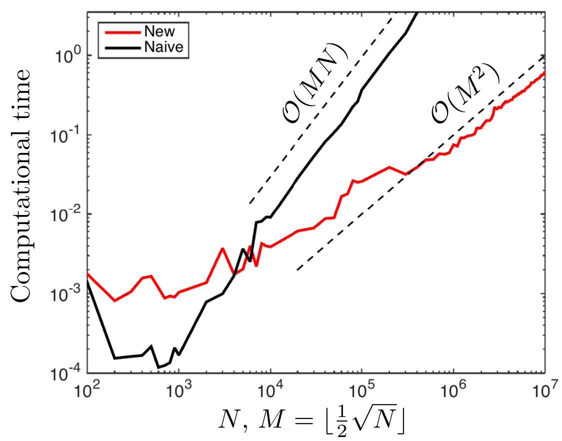

FIG. 5. *Computational times for constructing the normal equations in* (8) *when* $M = \lfloor \frac{1}{2}\sqrt{N} \rfloor$. *We compare the naive approach (black) that directly computes the matrix-matrix product* $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$ *and the approach (red) described in Section 7. While the naive approach has a theoretical complexity of* $\mathcal{O}(M^2N)$ *when* $M = \lfloor \frac{1}{2}\sqrt{N} \rfloor$, *the dominating computational cost for* $N < 10^6$ *is the* $\mathcal{O}(MN)$ *cost of evaluating* $\mathbf{T}_M(\underline{x}^{equi})$ *using a three-term recurrence.*

only $M+1$ possible values for $(m-n)^2$, $2M+1$ possible values of $(m+n)^2$, and at most $2M-1$ values of $1 \leq s \leq m+n-1$. This means that there are $\mathcal{O}(M^2)$ different products that appear in the set of formulas for $\widetilde{E}_{mn}$, $0 \leq m, n \leq M$, and these can be computed in a total of $\mathcal{O}(M^2)$ operations. In principle each $\widetilde{E}_{mn}$ for $0 \leq m, n \leq M$ sums up $\mathcal{O}(M)$ of these products weighted by Bernoulli numbers, requiring a total of $\mathcal{O}(M^3)$ operations to compute $\widetilde{E}$. However, the weighted Bernoulli numbers decay so rapidly to zero that we truncate the sums in (38) if $s > 10$. Therefore, we can compute $\widetilde{E}$ in $\mathcal{O}(M^2)$ operations. Once the matrix $\widetilde{E}$ is calculated the matrix $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})$ can immediately computed from (37).

For the Bernoulli numbers in (38) we tabulate $B_{s+1}/(s+1)!$ for $2 \leq s \leq 10$ and then use the first six terms in an asymptotic expansion for $s > 10$, i.e.,

$$\frac{B_{s+1}}{(s+1)!} \approx (-1)^{(s+3)/2} \frac{2}{(2\pi)^{s+1}} \left(1 + \frac{1}{2^{s+1}} + \frac{1}{3^{s+1}} + \frac{1}{4^{s+1}} + \frac{1}{5^{s+1}} + \frac{1}{6^{s+1}}\right), \quad s \text{ odd.}$$

This alleviates overflow issues with computing B_{s+1} and $(s+1)!$ separately when s is large.

Figure 5 shows the computational timings for constructing the normal equations, $\mathbf{T}_M(\underline{x}^{equi})^*\mathbf{T}_M(\underline{x}^{equi})\underline{c} = \mathbf{T}_M(\underline{x}^{equi})^*\underline{f}$, using the naive approach and the algorithm described in this section. When $M = \lfloor \frac{1}{2}\sqrt{N} \rfloor$ and $M > 50$, it is computationally more efficient to construct the normal equations using this new direct algorithm.

Acknowledgments. We wish to thank Mohsin Javed for his correspondence regarding the Euler–Maclaurin error formula in [25]. We also thank Ben Adcock for directing us to the literature on stable reconstruction and telling us about [4]. LD is grateful to AFOSR, ONR, NSF, and Total SA for funding.

Appendix A. Three applications of Gerschgorin's circle Theorem. Gerschgorin's circle Theorem can be used to bound the spectrum of a square matrix as it restricts the eigenvalues of a matrix A to the union of disks centered at the diagonal entries of A [22, p. 320].

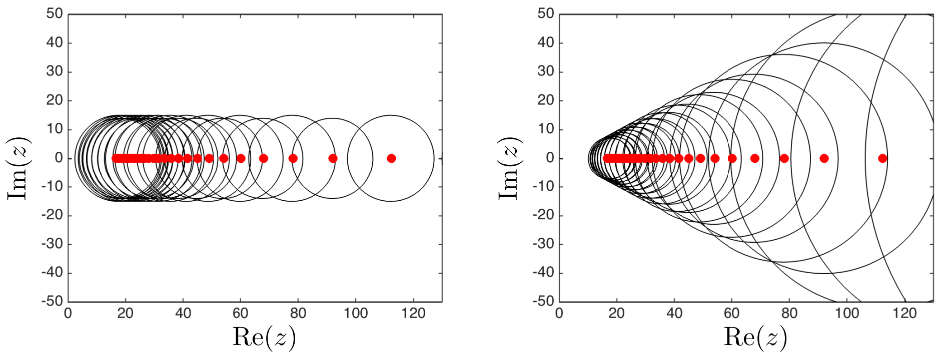

FIG. 6. *Left: The Gerschgorin disks for the matrix $D+C$ near $\mathrm{Re}(z)=0$ used in Lemma 17 when $N=1{,}000$ and $M=30$. Without a similarity transform the Gerschgorin circles give a poor lower bound on $\lambda_{M+1}(D+C)$. Right: The Gerschgorin disks for $P(D+C)P^{-1}$ near $\mathrm{Re}(z)=0$, where $P=\mathrm{diag}(D_{00},\ldots,D_{MM})$. The Gerschgorin disks now give a better lower bound on $\lambda_{M+1}(D+C)$. Another diagram shows that a similarity transform is not needed for bounding $\lambda_1(D+C)$.*

THEOREM 16. *Let $A \in \mathbb{C}^{n\times n}$ with entries a_{ij}. Then, the eigenvalues of A lie within at least one of the* Gerschgorin disks*,*

$$|z-a_{ii}| \leq \sum_{j=1,j\neq i}^{n} |a_{ij}|, \qquad 1 \leq i \leq n.$$

For a given square matrix A, the eigenvalue bounds given in Theorem 16 can be quite weak. A standard trick is to sharpen the bounds by using a carefully selected similarity transform. For any invertible matrix P the matrix PAP^{-1} has the same spectrum as A, but may have Gerschgorin disks with smaller radii and this can sharpen a bound on an eigenvalue of interest. Here, we apply Gerschgorin's circle Theorem to three matrices and select diagonal similarity transforms to improve the bounds.

First, we use Gerschogrin's circle Theorem to bound the spectrum of the matrix $D+C$ from Theorem 7. This result is used to then derive a bound on the singular values of $\mathbf{P}_M(\underline{x}^{equi})$. In Figure 6 we draw the Gerschgorin circles for $D+C$ and $P(D+C)P^{-1}$, where $P=\mathrm{diag}(D_{00},\ldots,D_{MM})$. It is this diagram that motivates the proof of the lemma below.

LEMMA 17. *For integers M and N satisfying $M \leq N$, let D be the diagonal matrix with entries $D_{mm}=N/(2m+1)$ for $0\leq m\leq M$ and C be the $(M+1)\times(M+1)$ matrix given in (17). The following bounds on the maximum and minimum eigenvalues hold:*

$$\lambda_1(D+C) \leq \frac{2N+M+3}{2}, \qquad \lambda_{M+1}(D+C) \geq \frac{N-\frac{1}{2}M^2}{2M+1}.$$

Proof. The matrix $D+C$ is symmetric so all the eigenvalues are real. By Theorem 16 applied to $D+C$ (without a similarity transform) we find that

$$\lambda_1(D+C) \leq \max_{0\leq j\leq M} \left\{ (D+C)_{jj} + \sum_{k=0,k\neq j}^{M} |C_{jk}| \right\} \leq N+1+\tfrac{M+1}{2},$$

as required. For λ_{M+1} we consider the matrix $P(D+C)P^{-1}$, where P is the diagonal matrix $\text{diag}(D_{00},\ldots,D_{MM})$. By Theorem 16 we have

$$\begin{aligned}\lambda_{M+1}(D+C) &\geq \min_{0\leq j\leq M}\left\{(P(D+C)P^{-1})_{jj} - \sum_{k=0,k\neq j}^{M}|(PCP^{-1})_{jk}|\right\}\\ &\geq \frac{N}{2M+1}+1-\frac{N}{2M+1}\frac{(M+1)(M+2)}{2N}\\ &\geq \frac{N-\frac{1}{2}M^2}{2M+1}+\frac{M}{2(2M+1)} \geq \frac{N-\frac{1}{2}M^2}{2M+1},\end{aligned}$$

as required. ∎

The second application of Gerschgorin's circle Theorem is on the matrix $F+C$ appearing in Theorem 8, where an upper bound on the maximum eigenvalue of $F+C$ is required. A similarity transform is not needed here.

LEMMA 18. *Let M and N be integers satisfying $M \leq N$. Let F be the matrix given in (23) and C be the $(M+1)\times(M+1)$ matrix given in (17). The following bound on the maximum eigenvalue holds:*

$$\lambda_1(F+C) \leq \frac{4N+M+1}{2}.$$

Proof. The matrix $F+C$ is symmetric so all the eigenvalues are real. By Theorem 16 applied to $D+C$ we have

$$\lambda_1(F+C) \leq \max_{0\leq j\leq M}\left\{(F+C)_{jj} + \sum_{k=0,k\neq j}^{M}|F_{jk}+C_{jk}|\right\} \leq 2N + \frac{M+1}{2},$$

as required. ∎

Lemma 17 and Lemma 18 are easy applications of Gerschgorin's circle Theorem; however, the next application is more technical. For Theorem 8, we want to bound $\|S\|_2$, where S is the change of basis matrix given in (22). It is also not clear if the Gerschgorin's circle Theorem is applicable here. Fortunately, S is a matrix with nonnegative entries so that it is possible to bound $\|S\|_2$ by the spectrum of its symmetric part [21].

Let $r(S) = \sup\left\{|v^*Sv| : v \in \mathbb{C}^{M\times 1}, v^*v = 1\right\}$ be the numerical range of S. Then, $\|S\|_2 \leq 2r(S)$. Since S has nonnegative entries we have [21, Thm. 1]

$$r(S) \leq \max\left\{|\lambda| : S^+v = \lambda v, v \neq 0\right\},$$

where $S^+ = (S+S^*)/2$ is the symmetric part of S. Therefore, we can use Gerschgorin's circle Theorem to bound $\max_{1\leq i\leq M+1}|\lambda_i(S^+)|$ and then use

$$\|S\|_2 \leq 2\max_{1\leq i\leq M+1}|\lambda_i(S^+)|. \tag{39}$$

It is technical to bound $\max_{1\leq i\leq M+1}|\lambda_i(S^+)|$ using Gerschgorin's circle Theorem. In Figure 7 we show the Gerschgorin's disk for S^+ and PS^+P^{-1}, where $P_{00}=1$ and $P_{ii}=\sqrt{i}$ for $i\geq 1$. The circles are tight if we work with PS^+P^{-1}.

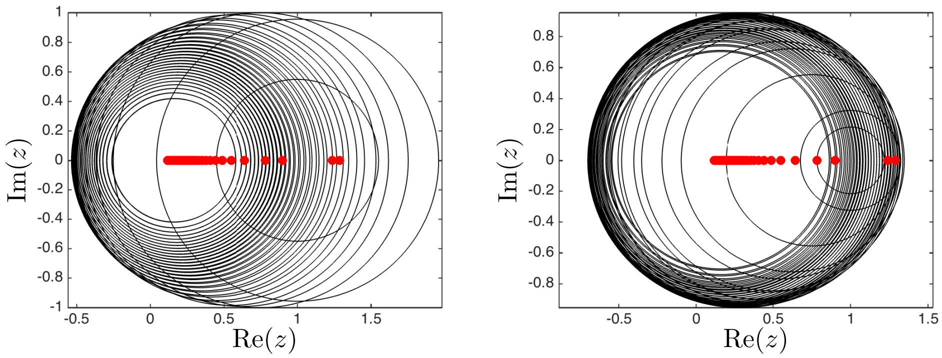

FIG. 7. *Left: The Gerschgorin disks for S^+ in Lemma 19 when $M = 50$. Without a similarity transform the Gerschgorin circles give a poor upper bound on $\lambda_1(S^+)$. Right: The Gerschgorin disks for $P(D+C)P^{-1}$, where $P = \operatorname{diag}(1, \sqrt{1}, \ldots, \sqrt{M})$. The Gerschgorin disks now provide a tight upper bound on $\lambda_1(S^+)$ as $M \to \infty$.*

LEMMA 19. *Let M be an integer and S^+ be the symmetric part of the $(M+1) \times (M+1)$ matrix S in (22). Then,*

$$\max_{1 \le i \le M+1} |\lambda_i(S^+)| \le \frac{5}{2}.$$

From (39) we conclude that $\|S\|_2 \le 5$.

Proof. We apply Theorem 16 to $A = PS^+P^{-1}$, where $P_{00} = 1$ and $P_{ii} = \sqrt{i}$ for $i \ge 1$. The entries of A are given explicitly by

$$A_{ij} = \begin{cases} 1, & i = j = 0, \\ \frac{1}{2\pi\sqrt{j}} \Psi(\frac{j}{2})^2, & i = 0, j > 0, j \text{ even}, \\ \frac{\sqrt{i}}{2\pi} \Psi(\frac{i}{2})^2, & j = 0, i > 0, i \text{ even}, \\ \frac{\sqrt{i}}{\pi\sqrt{j}} \Psi(\frac{j-i}{2}) \Psi(\frac{j+i}{2}), & i, j > 0, i + j \text{ even}, \end{cases} \qquad 0 \le i, j \le M,$$

where $\Psi(j) = \Gamma(j + 1/2)/\Gamma(j+1)$ and $\Gamma(x)$ is the Gamma function. We consider the Gerschgorin's disk in four cases: (1) the disk centered at A_{00}, (2) the disk centered at A_{11}, (3) the disks centered at A_{ii} with $i = 2k > 0$; and, (4) the disks centered at A_{ii} with $i = 2k+1 > 1$.

Case 1: The Gerschogrin disk centered at $\mathbf{A_{00}}$. First note that by Wendel's lower bound on the ratio of Gamma functions [35] we have

$$\Psi(j)^2 \le \frac{j+1}{(j+1/2)^2} \le \frac{1}{j}, \qquad j \ge 1. \tag{40}$$

Using (40) we can bound the radius of the Gerschogrin disk centered at A_{00} as follows:

$$\sum_{j=1}^{\lfloor M/2 \rfloor} A_{0,2j} \le \frac{1}{2\pi} \sum_{j=2}^{\infty} \frac{\Psi(j)^2}{\sqrt{2j}} \le \frac{1}{2\sqrt{2}\pi} \sum_{j=2}^{\infty} \frac{1}{j^{3/2}} = \frac{1}{2\sqrt{2}\pi} \left(\zeta(3/2) - 1\right) \le 0.19.$$

Since $A_{00} = 1$ the Gerschgorin disk is contained in $\{z \in \mathbb{C} : |z| \le 1.19\}$.

Case 2: The Gerschogrin disk centered at $\mathbf{A_{11}}$. Since $\Gamma(z+1) = z\Gamma(z)$ we have

$$\Psi(j+1) = \frac{j+1/2}{j+1}\Psi(j) \leq \Psi(j), \qquad j \geq 0,$$

and hence, $\Psi(0), \Psi(1), \Psi(2), \ldots$ is a monotonically decreasing sequence. Using this we can bound the radius of the Gerschogrin disk centered at A_{11} as follows:

$$\begin{aligned}\sum_{j=1}^{\lfloor M/2 \rfloor} A_{1,2j-1} &\leq \frac{1}{\pi\sqrt{3}}\Psi(1)\Psi(2) + \frac{1}{\pi}\sum_{j=3}^{\infty}\frac{\Psi(j-1)\Psi(j)}{\sqrt{2j-1}} \\ &\leq \frac{1}{\pi\sqrt{3}}\Psi(1)\Psi(2) + \frac{\sqrt{2}}{2\pi}(\zeta(3/2)-1) \leq 0.48,\end{aligned}$$

where we used $\Psi(j-1)\Psi(j) \leq \Psi(j)^2 \leq j^{-1} \leq (j-1)^{-1}$ and $(2j-1)^{-1/2} \leq \sqrt{2}j^{-1/2}$. Since $A_{11} = 1$ the Gerschgorin disk is contained in $\{z \in \mathbb{C} : |z| \leq 1.48\}$.

Case 3: The Gerschogrin disks centered at $\mathbf{A_{ii}}$ with $\mathbf{i = 2k > 0}$. The radii of the Gerschgorin disks centered at A_{ii} with $i = 2k > 0$ is bounded by

$$\begin{aligned}\sum_{j=0, j\neq k}^{\lfloor M/2 \rfloor} A_{2k,2j} \leq \underbrace{\frac{1}{2\pi}\Psi(k)^2(2k)^{\frac{1}{2}}}_{=(1)} + \underbrace{\frac{1}{\pi}\sum_{j=1}^{k-1}\Psi(k-j)\Psi(k+j)\left(\frac{k}{j}\right)^{\frac{1}{2}}}_{=(2)} \\ + \underbrace{\frac{1}{\pi}\sum_{j=k+1}^{\infty}\Psi(j-k)\Psi(j+k)\left(\frac{k}{j}\right)^{\frac{1}{2}}}_{=(3)}.\end{aligned}$$

We bound the three parts in turn. By (40) we have

$$(1) \leq \frac{1}{2\pi}\Psi(k)^2(2k)^{\frac{1}{2}} \leq \frac{\sqrt{2}}{2\pi}k^{-1/2} \leq 0.23.$$

Next, note that $(2) = 0$ if $k = 1$ so we can assume that $k \geq 2$. For $k \geq 2$, the summands in (2) have a single local minimum. For small j the terms in (2) are monotonically decreasing and for larger j are monotonically increasing. This means we can apply a double-sided integral test to bound the sum. That is,

$$(2) \leq \frac{1}{\pi}\Psi(1)\Psi(2k-1)\frac{k^{1/2}}{(k-1)^{1/2}} + \frac{1}{\pi}\Psi(k-1)\Psi(k+1)k^{1/2} + \frac{1}{\pi}\int_1^{k-1}\frac{\sqrt{k}}{\sqrt{(k-x)x(x+k)}}dx. \tag{41}$$

Since $\Psi(1) = \sqrt{\pi}/2$, $\Psi(2k-1) \leq (2k-1)^{-1/2}$, $\Psi(k-1)\Psi(k+1)k^{1/2} \leq k^{-1/2}$, and the fact that the continuous integral in (41) can be expressed in terms of a hypergeometric function, we have

$$\begin{aligned}(2) &\leq \frac{k^{-1/2}}{\pi} + \frac{1}{2\sqrt{\pi}}\left(\frac{k}{(k-1)(2k-1)}\right)^{\frac{1}{2}} + \frac{2}{\pi\sqrt{k}}\,{}_2F_1(\tfrac{1}{4}, \tfrac{1}{2}, \tfrac{5}{4}; (1-k^{-1})^2) \\ &\leq \frac{1}{\sqrt{2}\pi} + \frac{\sqrt{3}}{2\sqrt{2\pi}} + \frac{1.03}{2\sqrt{2\pi}} \leq 0.78.\end{aligned} \tag{42}$$

Here, in the penultimate inequality we used $k^{-1/2} \leq 1/\sqrt{2}$ for $k \geq 2$, $k/(k-1)(2k-1) \leq 2/3$ for $k \geq 2$, and ${}_2F_1(\frac{1}{4}, \frac{1}{2}, \frac{5}{4}; (1-k^{-1})^2) \leq {}_2F_1(\frac{1}{4}, \frac{1}{2}, \frac{5}{4}; \frac{1}{4}) \leq 1.03$ for $k \geq 2$.

Finally, for (3) we note that the summands are monotonically decreasing so that by the integral bound we have

$$(3) \leq \frac{1}{\pi}\Psi(1)\Psi(2k+1)\left(\frac{k}{k+1}\right)^{\frac{1}{2}} + \frac{1}{\pi}\int_{k+1}^{\infty} \frac{\sqrt{k}}{\sqrt{(x-k)x(x+k)}}dx.$$

Since $\Psi(1) = \sqrt{\pi}/2$, $\Psi(2k+1)^2 \leq 1/(2k+1)$, and the continuous integral can be transformed into a elliptic integral (of the first kind), denoted by F, we have

$$\begin{aligned}(3) &\leq \frac{1}{2\sqrt{\pi}}\left(\frac{k}{(k+1)(2k+1)}\right)^{1/2} + \frac{2}{\pi}F\left(\sin^{-1}\left(\sqrt{\tfrac{k}{k+1}}\right), -1\right) \\ &\leq \frac{1}{2\sqrt{6\pi}} + \frac{\Gamma(1/4)^2}{2\sqrt{2}\pi^{3/2}} \leq 0.95.\end{aligned} \tag{43}$$

Here, in the penultimate inequality we used $k/((k+1)(2k+1)) \leq 1/6$ for $k \geq 1$ and $F(\sin^{-1}(\sqrt{k/(k+1)}), -1) \leq F(\pi/2, -1) = \Gamma(1/4)^2/(4\sqrt{2\pi})$.

Since $|A_{ii}| \leq A_{22} \leq 3/8$ for $i \geq 2$ and $3/8 + 0.23 + 0.78 + 0.95 \leq 2.34$, these Gerschgorin disks are contained in $\{z \in \mathbb{C} : |z| \leq 2.34\}$.

Case 4: The Gerschogrin disks centered at $\mathbf{A_{ii}}$ with $\mathbf{i = 2k+1 > 1}$. The radii of a Gerschgorin disk centered at A_{ii} with $i = 2k+1 > 0$ is bounded by

$$\sum_{j=0, j\neq k}^{\lfloor M/2 \rfloor} A_{2k+1,2j+1} \leq \underbrace{\frac{1}{\pi}\sum_{j=1}^{k-1}\Psi(k-j)\Psi(k+j+1)\left(\frac{2k+1}{2j+1}\right)^{\frac{1}{2}}}_{=(i)} + \underbrace{\frac{1}{\pi}\sum_{j=k+1}^{\infty}\Psi(j-k)\Psi(j+k+1)\left(\frac{2k+1}{2j+1}\right)^{\frac{1}{2}}}_{=(ii)}.$$

Since $\Psi(j+k+1) \leq \Psi(j+k)$ and $(2k+1)/(2j+1) \leq k/j$ for $1 \leq j \leq k-1$, we have from (42)

$$(i) \leq \frac{1}{\pi}\sum_{j=1}^{k-1}\Psi(k-j)\Psi(k+j)\left(\frac{k}{j}\right)^{\frac{1}{2}} \leq 0.78.$$

Moreover, since $\Psi(j+k+1) \leq \Psi(j+k)$ and $(2k+1)/(2j+1) \leq 2k/j$ for $j \geq k+1$, we have from (43)

$$(ii) \leq \frac{\sqrt{2}}{\pi}\sum_{j=k+1}^{\infty}\Psi(j-k)\Psi(j+k)\left(\frac{k}{j}\right)^{\frac{1}{2}} \leq 0.95 \times \sqrt{2} \leq 1.35.$$

Since $|A_{ii}| \leq A_{33} \leq 5/16$ for $i \geq 3$ and $5/16 + 0.78 + 1.35 \leq 2.45$, these Gerschgorin disks are contained in $\{z \in \mathbb{C} : |z| \leq 2.45\}$.

By Theorem 16 we conclude that $\max_{1 \leq i \leq M+1} |\lambda_i(S^+)| \leq 2.45 < 5/2$. ◻

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