HOW WELL-CONDITIONED CAN THE EIGENVALUE PROBLEM BE?

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ABSTRACT. The condition number for eigenvalue computations is a well-studied quantity. But how small can we expect it to be? Namely, which is a perfectly conditioned matrix w.r.t. eigenvalue computations? In this note we answer this question with exact first order asymptotic.

1. INTRODUCTION AND RESULT

For a matrix $A \in \mathbb{C}^{n \times n}$ and an eigenpair $(\lambda, x) \in \mathbb{C} \times \mathbb{C}^n$, the classical Schur decomposition yields an unitary matrix Q such that

(1)
$$Q^H A Q = \begin{pmatrix} \lambda & w^H \\ 0 & B \end{pmatrix},$$

where \cdot^{H} denotes the Hermitian conjugate and $w \in \mathbb{C}^{n-1}$ is a vector. Denoting by $y \in \mathbb{C}^{n}$ the corresponding left eigenvector, the condition numbers for the eigenvalue λ and eigenvector x are given by (see for example [5])

$$\kappa_{\lambda}(A) = \frac{\|y\| \, \|x\|}{|y^H x|} \quad \text{and} \quad \kappa_x(A) = \frac{1}{\sigma_{\min}(B - \lambda \cdot \mathrm{Id}_{(n-1) \times (n-1)})}$$

where σ_{\min} denotes the least singular value and Id is the identity matrix. In other words, if we allow for a ε -size perturbation of A, the eigenpair $(\hat{\lambda}, \hat{x})$ of the perturbed matrix will satisfy

$$|\hat{\lambda} - \lambda| \le \varepsilon \kappa_{\lambda}(A) + O(\varepsilon^2), \quad \angle(x, \hat{x}) \le \varepsilon \kappa_x(A) + O(\varepsilon^2).$$

If the matrix $A \in \mathbb{C}^{n \times n}$ is diagonal with pairwise different entries z_1, \ldots, z_n , we have $\kappa_{z_i}(A) = 1$ for all *i* and the eigenvector condition number admits a simpler expression

$$\kappa_{e_i}(A) = \frac{1}{\min_{j \neq i} |z_i - z_j|}.$$

In this note we investigate the following natural question: how good can the eigenvector conditioning of a $n \times n$ matrix be? The answer has a concrete application in the search for good starting points for homotopy methods for the eigenvector problem, see [1], but it is just such a natural and basic question that it deserves an

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answer on its own right! The answer is not trivial. For example, if $A = Id_{n \times n}$ we clearly have $\kappa_x(A) = \infty$ (and it is a rather well–known fact that one can perturb the identity matrix $Id_{n \times n}$ with very small changes to get any desired collection of eigenvectors). In general, one is interested in perturbations which are relative to the size of A, that is, perturbations of size $\varepsilon ||A||_*$ where $||A||_*$ is either the operator or the Frobenius norm.

Problem. Which is the optimal value for the relative–error perturbation eigenvector conditioning of $A \in \mathbb{C}^{n \times n}$, that is, which matrix minimizes the quantity

$$\kappa_{\max,*}(A) = \max_{x} \left(\kappa_x(A) \|A\|_* \right)$$

where x runs over all eigenvectors of A and $||A||_* = ||A||_{\text{Frob}}$ or $||A||_* = ||A||_{\text{op}}$ is the Frobenius or the operator norm?

We recall the unit–side triangular (sometimes called hexagonal!) lattice in $\mathbb{C} \equiv \mathbb{R}^2$ which is the set of points of the form



FIGURE 1. An extremal configuration (to leading order): a circle at the origin and the points of a triangular lattice inside the circle.

Our main result states that the diagonal matrix whose entries range over the triangular lattice, solves Problem 1, at least with respect to the leading order term.

Theorem. Let $\{z_1, \ldots, z_n\} \subset \mathbb{C}^n$ be first *n* points in the unit-side triangular lattice, in increasing modulus order (if two points have the same modulus, we take any of them). Then, as $n \to +\infty$,

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$$\kappa_{\max,\operatorname{Frob}}(\operatorname{Diag}(z_1,\ldots,z_n)) = \frac{3^{1/4}}{2\sqrt{\pi}}n + o(n),$$

$$\kappa_{\max,\operatorname{op}}(\operatorname{Diag}(z_1,\ldots,z_n)) = \frac{3^{1/4}}{\sqrt{2\pi}}\sqrt{n} + o(\sqrt{n}).$$

Moreover, this diagonal matrix is asymptotically optimal in the sense that for any matrix $A \in \mathbb{C}^{n \times n}$ the equalities above give lower bounds for $\kappa_{\max, Frob}$ and $\kappa_{\max, op}$.

It would naturally be interesting to have a better understanding of the error terms and, in particular, to have a better understanding of the extremal configurations. We believe it to be conceivable that our construction may perhaps be quite close to optimal even with respect to lower order error terms. For a configuration minimizing the Frobenius norm it is clear that the center of mass has to be at 0. This can of course be achieved by a translation of less than unity and does not affect the asymptotic main term. In order to get the Theorem, we will prove the following asymptotic inequality which is interesting on its own right.

Proposition. Let p > 0 be fixed. We have, for any $z_1, \ldots, z_n \in \mathbb{C}$, as $n \to \infty$,

$$\frac{1}{\min_{i\neq j}|z_i - z_j|} \left(\sum_{i=1}^n |z_i|^p\right)^{1/p} \ge \left(\frac{2}{p+2}\right)^{1/p} \frac{3^{1/4}}{\sqrt{2\pi}} n^{\frac{1}{2} + \frac{1}{p}} + o\left(n^{\frac{1}{2} + \frac{1}{p}}\right),$$

and this bound is matched by z_1, \ldots, z_n as in the Theorem.

Just as in the Theorem, it might be interesting to get a better understanding of the lower-order terms. If optimal configurations are indeed close to a subset of the hexagonal lattice, then this is strongly related to the Gauss Circle Problem and these techniques might apply (we observe that the function $z \to |z|^p$ is also smoother than the cut-off function used in the Gauss circle problem).

2. Proofs

§2.1. gives a proof of the Theorem (assuming the Proposition). Section 2.2 contains a simple geometric Lemma, the proof of the Proposition is given in Section 2.3.

2.1. Proof of the Theorem.

Proof. From (1) it is clear that the eigenvector conditioning of a matrix is invariant under conjugation by unitary matrices. From the Schur decomposition, we can thus assume that A is upper-triangular. Now, for any eigenvector x the definition of $\kappa_x(A)$ does not involve w in (1), but w contributes to the norm $||A||_*$, so the value of $\kappa_{\max,*}$ does not grow by setting w = 0 for all eigenvectors. It follows that the matrix with optimal value of $\kappa_{\max,*}$ can be chosen diagonal (of course, conjugating it by any unitary matrix we get a normal matrix with identical conditioning). Thus, to prove the last claim of the Theorem we can assume that A is diagonal, but in this case we note that

$$\kappa_{\max, \text{Frob}}(\text{Diag}(z_1, \dots, z_n)) = \max_{i \neq j} \frac{\|(z_1, \dots, z_n)\|_2}{|z_i - z_j|},$$

$$\kappa_{\max, \text{op}}(\text{Diag}(z_1, \dots, z_n)) = \max_{i \neq j} \frac{\|(z_1, \dots, z_n)\|_{\infty}}{|z_i - z_j|},$$

and the result is immediate from Proposition 1 for the cases p = 2 and $p = \infty$. \Box

2.2. A Lemma. We denote a ball of radius r centered in the origin by

$$B_r = \{ z \in \mathbb{C} : |z| < r \}.$$

We say that a set $\{z_1, \ldots, z_n\} \subset \mathbb{C}$ is 1-separated if, for all $i \neq j$

$$|z_i - z_j| \ge 1.$$

We also introduce the counting function $N : [0, \infty] \to \mathbb{N}$ as follows: N(r) is the cardinality of the largest possible 1-separated set contained in B_r . This quantity was already studied by L. Fejes Tóth in 1940 who determined its growth.

Lemma 1 (Fejes Tóth [2]). We have, as $r \to +\infty$,

$$N(r) = \frac{2\pi}{\sqrt{3}}r^2 + o(r^2).$$

Equality is attained for the unit-side triangular lattice in B_r .

We give a simple sketch why this would be the case – the simple geometric argument makes use of Apollonian Circle Packings and the well-understood fact that the asymptotically densest packing of circles in the plane is given by the hexagonal lattice (which, not entirely coincidentally, is also a result of Fejes Tóth [3]).

Sketch of Proof. The claim on the triangular lattice (which implies the lower bound for the equality in the lemma) follows from [4, Eq. (1.6)]: for any lattice $L \subset \mathbb{R}^2$ (given by the set of points of the form $T\binom{a}{b}$ with $T \in \mathbb{R}^{2 \times 2}$ and $a, b \in \mathbb{Z}$,

$$#\{L \cap B_r\} = \frac{\pi r^2}{\det(T)} + O(r^{\frac{1}{3}}\sqrt{\log r}), \quad r \to +\infty.$$

In the case of the triangular lattice, $\det(T) = \sqrt{3}/2$ and we get the desired result. As for the upper bound, we argue by contradiction. Suppose that there exists $\varepsilon > 0$ such that there exists a divergent sequence $(r_n) \to \infty$ such that

$$N(r_n) \ge \left(\frac{2\pi}{\sqrt{3}} + \varepsilon\right) r_n^2$$

Let us pick a sufficiently large r_n and let us tile \mathbb{R}^2 using balls of radius r_n in the fashion of a square or hexagonal lattice (it does not really matter). This allows us to cover a large amount of space with very efficient 1-separated point sets.



FIGURE 2. Using more disks with smaller radii allows for more precise approximation.

We then refine the disk packing by packing disks of smaller radius (see Fig. 2) between the big balls and use a standard hexagonal lattice to fill those disks. We can iterate this construction until we capture $\sim 1-$ of the entire plane. Not that, since r_n can be chosen to be arbitrarily large, this can always be done with a finite number of steps only depending on ε . However, this then allows us to generate a period packing of disks whose asymptotic density exceeds $\pi/\sqrt{12}$ which is a contradiction.

2.3. Proof of the Proposition.

Proof. Let p > 0 and let $\{z_1, \ldots, z_n\} \subset \mathbb{R}^2$ be a 1-separated set. Our goal is to prove a lower bound on

the quantity
$$\frac{1}{\min_{i \neq j} |z_i - z_j|} \left(\sum_{i=1}^n |z_i|^p\right)^{1/p}.$$

We use invariance under dilation to assume without loss of generality that

$$\min_{i \neq j} |z_i - z_j| = 1$$

and this will be assumed in all subsequent arguments. We abbreviate

$$M = \max_{1 \le i \le n} |z_i|$$

and write

$$\sum_{i=1}^{n} |z_i|^p = p \sum_{i=1}^{n} \int_0^{|z_i|} y^{p-1} \, dy$$

= $p \int_0^M y^{p-1} \cdot \# \{ 1 \le i \le n : |z_i| > y \} \, dy$
= $p \int_0^M y^{p-1} \cdot (n - \# \{ 1 \le i \le n : |z_i| \le y \}) \, dy$
 $\ge p \int_0^M y^{p-1} \max(n - N(y), 0) \, dy.$

Now, by the Lemma (or the theorem given in [2]) for every $\varepsilon > 0$ there is an n_0 such that for every $n \ge n_0$

(2)
$$M > \frac{3^{1/4} - \varepsilon}{\sqrt{2\pi}} \sqrt{n}.$$

From this we derive

$$\begin{split} \sum_{i=1}^{n} |z_i|^p &\geq p \int_0^{\frac{3^{1/4} - \varepsilon}{\sqrt{2\pi}}\sqrt{n}} y^{p-1} \max\left(n - \frac{2\pi}{\sqrt{3}}y^2 + o(y^2), 0\right) \, dy \\ &= \left(\frac{3^{1/4} - \varepsilon}{\sqrt{2\pi}}\sqrt{n}\right)^p \left(1 - \frac{p}{p+2} \frac{(3^{1/4} - \varepsilon)^2}{\sqrt{3}}\right) n + o\left(n^{\frac{p+2}{2}}\right), \end{split}$$

which implies the proposition. For $p = \infty$, the assertion is just equation (2). By observing that the bounds used for N(r) are sharp to leading order for the hexagonal lattice, we see that all the inequalities are asymptotically sharp.

However, there is also a direct geometric argument, valid for p > 1, using the construction in [1, Lemma 2.27]: For any given n, we take the first n points in the unit-side triangular lattice, with increasing norm (if two points have the same norm, we take any of them). We first note that the function $z \to |z|^p$ is convex, hence by Jensen's inequality, for any regular hexagon H centered at z_i we have

$$\mathbb{E}_{z \in H}(|z|^p) \ge |\mathbb{E}_{z \in H}(z)|^p = |z_i|^p,$$

where \mathbb{E} has to be understood as the expected value in the hexagon. Since by construction the points are in the unit-side triangular lattice, the Voronoi cells surrounding each z_i is a hexagon H_i and we thus have

$$\sum_{i=1}^{n} |z_i|^p \le \sum_{i=1}^{n} \mathbb{E}_{z \in H_i}(|z|^p) = \frac{1}{\operatorname{vol}(H)} \int_{\bigcup_i H_i} |z|^p \, dz.$$

(note that all the hexagons have the same area, which we denote by $vol(H) = \sqrt{3}/2$). Now, from the Lemma it follows that in the disk of radius r there are at least $2\pi r^2/\sqrt{3} + O(r^{1/3}\sqrt{\log r})$ points of the unit-side triangular lattice. Therefore, it follows that all the H_i are contained in a disk of radius $r_n := 3^{1/4}\sqrt{n}/\sqrt{2\pi} + o(n)$,

which yields

$$\sum_{i=1}^{n} |z_i|^p \le \frac{1}{\operatorname{vol}(H)} \int_{|z| \le r_n} |z|^p dz$$
$$= \frac{2\pi r_n^{p+2}}{(p+2)\operatorname{vol}(H)} = \frac{4\pi 3^{\frac{p+2}{4}}}{\sqrt{3}(p+2)(2\pi)^{1+p/2}} n^{1+p/2} + o(n^{1+p/2}),$$

which proves the upper bound.

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