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Numerical investigation of Crouzeix's conjecture

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ABSTRACT

Crouzeix's conjecture states that for all polynomials p and matrices A, the inequality $\|p(A)\| \leq 2\,\|p\|_{W(A)}$ holds, where the quantity on the left is the 2-norm of the matrix $p(A)$ and the norm on the right is the maximum modulus of the polynomial p on $W(A)$, the field of values of A. We report on some extensive numerical experiments investigating the conjecture via nonsmooth minimization of the Crouzeix ratio $f \equiv \|p\|_{W(A)}/\|p(A)\|$, using Chebfun to evaluate this quantity accurately and efficiently and the BFGS method to search for its minimal value, which is 0.5 if Crouzeix's conjecture is true. Almost all of our optimization searches deliver final polynomial-matrix pairs that are very close to nonsmooth stationary points of f with stationary value 0.5 (for which $W(A)$ is a disk) or smooth stationary points of f with stationary value 1 (for which $W(A)$ has a corner). Our observations have led us to some additional conjectures as well as some new theorems. We hope that these give insight into Crouzeix's conjecture, which is strongly supported by our results.

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1. Crouzeix's conjecture

Let $\mathcal{M}^n$ denote the space of $n \times n$ complex matrices, let $\mathcal{P}_m$ denote the space of polynomials with complex coefficients and degree $\leq m$, and let $\|\cdot\|$ denote the 2-norm. For $A \in \mathcal{M}^n$, the field of values (or numerical range) of A is

$$W(A) = \{v^*Av : v \in \mathbb{C}^n, \|v\| = 1\} \subset \mathbb{C}.$$

The Toeplitz–Hausdorff theorem states that $W(A)$ is convex for all $A \in \mathcal{M}^n$ [18, Ch 1].

Let $p \in \mathcal{P}_m$ and let $A \in \mathcal{M}^n$. In 2004, M. Crouzeix conjectured [8] that for all m and n,

$$\|p(A)\| \leq 2\,\|p\|_{W(A)}. \tag{1}$$

The left-hand side is the 2-norm (spectral norm, maximum singular value) of the matrix $p(A)$, while $\|p\|_{W(A)}$ on the right-hand side is $\max_{\zeta \in W(A)} |p(\zeta)|$. By the maximum modulus theorem, $\|p\|_{W(A)}$ must be attained on bd $W(A)$, the boundary of $W(A)$.

In 2007, Crouzeix proved [9] that

$$\|p(A)\| \leq 11.08\,\|p\|_{W(A)} \tag{2}$$

i.e., the conjecture is true if we replace 2 by 11.08. Crouzeix wrote:

> The estimate 11.08 is not optimal. There is no doubt that refinements are possible which would decrease this bound. We are convinced that our estimate is very pessimistic, but to improve it drastically (recall that our conjecture is that 11.08 can be replaced by 2), it is clear that we have to find a completely different method.

The example

$$p(\zeta) = \zeta - \lambda,\ A = \begin{bmatrix} \lambda & \alpha \\ 0 & \lambda \end{bmatrix},$$

where $\alpha, \lambda \in \mathbb{C}$, $\alpha \neq 0$, shows that 11.08 cannot be replaced by a *smaller* number than 2. In this case, $W(A)$ is the disk of radius $|\alpha|/2$ centered at λ so $\|p\|_{W(A)} = |\alpha|/2$, and $\|p(A)\| = |\alpha|$.

As the degree of p is unbounded in Crouzeix's conjecture (1) and theorem (2), they can be extended from polynomials to functions analytic in the interior of $W(A)$ and continuous on its boundary. This is because $W(A)$ is a compact subset of the complex plane such that $\mathbb{C}\backslash W(A)$ is connected, and by Mergelyan's theorem [24,25] any function analytic on the interior of such a set and continuous on its boundary can be uniformly approximated by polynomials. The conjecture and theorem can also be extended from matrix space to infinite-dimensional Hilbert space, where the only difference is that $W(A)$

may not be closed, so $\|p\|_{W(A)}$ is defined as $\sup_{\zeta \in W(A)} |p(\zeta)|$. Crouzeix's conjecture and theorem might seem somewhat esoteric, but in our view they are quite fundamental with remarkably broad impact: the norm of an analytic function of a matrix A is bounded by a modest constant times its norm on the field of values of A. Applications of the conjecture include estimating the transient behavior of $\|e^{tA}\|$ [15] and describing the convergence rate of GMRES [4].

The conjecture is known to hold for certain restricted classes of polynomials $p \in \mathcal{P}_m$ or matrices $A \in \mathbb{C}^{n \times n}$. Let $\mathcal{D}$ denote the open unit disk, and let $\overline{\mathcal{D}}$ denote its closure.

- $p(\zeta) = \zeta^m$ (from the power inequality [1,27], which states that the numerical radius $r(A^m)$ is less than or equal to $[r(A)]^m$, and since $\|A^m\| \le 2r(A^m)$, it follows that $\|A^m\| \le 2[r(A)]^m = 2\max_{\zeta \in W(A)} |\zeta^m|$)
- $W(A)$ is a disk (Badea [8, p. 462], based on von Neumann's inequality [29], which states that if B is a contraction, i.e., $\|B\| \le 1$, then $\|p(B)\| \le \sup_{\zeta \in \mathcal{D}} |p(\zeta)|$, and work of Okubo and Ando [26], which shows that if $r(A) \le 1$, then A is similar to a contraction B via a similarity transformation with condition number at most 2, and hence $\|p(A)\| \le 2\|p(B)\|$, giving the result when $W(A) = \overline{D}$; the extension to any disk follows by scaling and translating A)
- $n = 2$ (Crouzeix [8])
- the minimum polynomial of A has degree 2 (combining the previous result with [28])
- $n = 3$ and $A^3 = 0$ (Crouzeix [10] argues that the conjecture holds in this case using a combination of mathematical and numerical arguments)
- A is an upper Jordan block with a perturbation in the bottom left corner (Greenbaum and Choi [14]) or any diagonal scaling of such A (Choi [6])
- A is diagonalizable with an eigenvector matrix having condition number less than or equal to 2 (easy)
- $AA^* = A^*A$ (then the constant 2 can be improved to 1).

In the summer of 2016, César Palencia announced a surprising improvement over (2), namely

$$\|p(A)\| \le \left(1 + \sqrt{2}\right) \|p\|_{W(A)}. \tag{3}$$

A proof has recently appeared in [12].

2. The boundary of the field of values

It is well known from Kippenhahn [20] and Johnson [19] that bd $W(A)$, the boundary of $W(A)$, can be characterized as

$$\text{bd } W(A) = \{z_\theta = v_\theta^* A v_\theta : \theta \in [0, 2\pi)\} \tag{4}$$

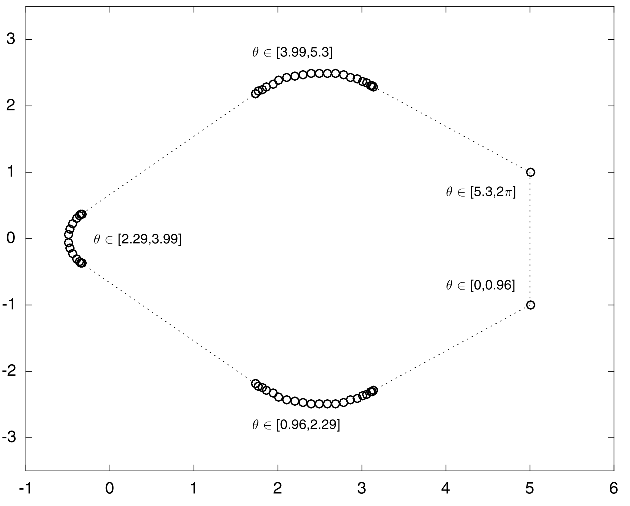

Fig. 1. For $A = \mathrm{diag}(J, B, D)$, the extreme points of $W(A)$ lie in the union of five connected sets, including the two eigenvalues $5 \pm i$.

where v_θ is a normalized eigenvector corresponding to the largest eigenvalue of the Hermitian matrix

$$H_\theta = \frac{1}{2}\left(e^{i\theta}A + e^{-i\theta}A^*\right).$$

The proof uses a supporting hyperplane argument (for a succinct version, see [16]).

As an example, let i denote the imaginary unit and let

$$J = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix},\ B = \begin{bmatrix} 1 & 2 \\ -3 & 4 \end{bmatrix},\ D = \begin{bmatrix} 5+i & 0 \\ 0 & 5-i \end{bmatrix}, A = \mathrm{diag}(J, B, D).$$

The fields of values of J, B and D are, respectively, the disk of radius $1/2$ centered at 0, an elliptical disk with major axis joining $2.5 \pm 2.5i$, and the line segment joining $5 \pm i$, and the field of values of A is the convex hull of these three sets. Fig. 1 plots the points $z_\theta \in \mathrm{bd}\, W(A)$ (shown as small circles) for some values of θ in $[0, 2\pi]$. The extreme points of $W(A)$ (those that cannot be expressed as a convex combination of two other points in the set) consist of five disjoint separated connected sets, two of which are the eigenvalues $5 \pm i$. The boundary of $W(A)$ also includes five line segments joining these sets, because the largest eigenvalue of H_θ has multiplicity two at five critical values of θ, and hence the corresponding eigenvector v_θ can be taken as any normalized vector in a two-dimensional subspace, resulting in multiple values for z_θ.

A point $z \in \mathrm{bd}\, W(A)$ is called a vertex (or a corner point, or a singular point) if there is more than one supporting hyperplane (supporting line) for $W(A)$ passing through z. It is known [20, Theorem 13] that vertices of $W(A)$ are always eigenvalues of A, such as $5 \pm i$ in Fig. 1. Clearly, bd $W(A)$ is nonsmooth at a vertex. Although the points in the interior of line segments of bd $W(A)$ cannot easily be parametrized by z_θ, due to its non-unique values, there is a convenient parametrization for these points which is based on computing the skew-Hermitian part of $e^{i\theta}A$ as well as its Hermitian part H_θ. Although this is not difficult to derive, it does not seem to be well known; the only reference we know is an unpublished paper by Cowen and Harel [5].

3. The Crouzeix ratio and its gradient

Let us identify $p \in \mathcal{P}_m$ with its coefficient vector $c = [c_0, c_1, \ldots, c_m]^T \in \mathbb{C}^{m+1}$, and define the function $q\colon \mathbb{C}^{m+1} \times \mathbb{C} \to \mathbb{C}$ by

$$q(c, \zeta) = \sum_{j=0}^{m} c_j \zeta^j.$$

We define the *Crouzeix ratio* as

$$f(c, A) = \frac{\tau(c, A)}{\beta(c, A)} \tag{5}$$

where

$$\tau(c, A) = \max\big\{|q(c, z)| : z \in W(A)\big\},$$

and

$$\beta(c, A) = \|p(A)\| = \sigma_{\max}\big(q(c, A)\big),$$

the largest singular value of $\sum_{j=0}^{m} c_j A^j$. Thus f maps the Euclidean space $\mathbb{C}^{m+1} \times \mathcal{M}^n$, with real inner product

$$\langle (c, A), (d, B) \rangle = \mathrm{Re}\big(c^* d + \mathrm{tr}(A^* B)\big), \tag{6}$$

to $\mathbb{R}$. Here $*$ denotes complex conjugate transpose. The notations τ and β were chosen to indicate the “top” and “bottom” components of the ratio. The conjecture (1) states that $f(c, A)$ is bounded below by 0.5 independently of the polynomial degree m and the matrix order n.

The Crouzeix ratio f is not convex, and it is not defined if the denominator is zero, but it is locally Lipschitz on the set of all pairs (c, A) for which $q(c, A) \neq 0$. It is semialgebraic (its graph is a finite union of sets, each of which is defined by a finite system of polynomial inequalities). It is a nonsmooth function, meaning that it is not differentiable at some points, which necessarily form a set of measure zero both because f is locally Lipschitz and because it is semialgebraic.

There are three different potential sources of nonsmoothness in the Crouzeix ratio f. The first occurs when the numerator $\tau(c, A)$ is attained at more than one point $z \in$

bd $W(A)$. The second possibility is that although $\tau(c, A)$ is attained only at a single point $z \in$ bd $W(A)$, the equation $z = v^*Av$ in (4) holds for two or more linearly independent unit vectors v. The third possibility is that the maximum singular value of $q(c, A)$, which defines the denominator of the Crouzeix ratio, has multiplicity two or more.

Theorem 1. *Suppose that $\tau(c, A)$ is attained at a unique point $z \in$ bd $W(A)$, that $z = v^*Av$ holds only for one unit vector v up to multiplication by a unimodular scalar, and that the maximum singular value of $q(c, A)$ is simple, with corresponding left and right singular vectors u and w satisfying $q(c, A)w = \beta(c, A)u$ and $u^*q(c, A) = \beta(c, A)w^*$, so that none of the three nonsmooth scenarios described above occur. Then the Crouzeix ratio f is differentiable at (c, A), and its gradient, w.r.t. the inner product (6), is*

$$\nabla f(c, A) = \frac{\beta(c, A)\nabla\tau(c, A) - \tau(c, A)\nabla\beta(c, A)}{\beta(c, A)^2} \tag{7}$$

where $\nabla\tau(c, A) = [\nabla_c\tau(c, A); \nabla_A\tau(c, A)]$, $\nabla\beta(c, A) = [\nabla_c\beta(c, A); \nabla_A\beta(c, A)]$, with

$$\nabla_c\tau(c, A) = \frac{q(c, z)}{|q(c, z)|}\left[1, \bar{z}, \ldots, \bar{z}^m\right]^T,$$

$$\nabla_A\tau(c, A) = \frac{q(c, z)}{|q(c, z)|}\sum_{j=1}^{m} j\bar{c}_j\bar{z}^{j-1}vv^*,$$

$$\nabla_c\beta(c, A) = \left[w^*u, w^*A^*u, \ldots, w^*(A^*)^m u\right]^T,$$

$$\nabla_A\beta(c, A) = \sum_{j=1}^{m}\sum_{\ell=0}^{j-1}\bar{c}_j(A^*)^\ell uw^*(A^*)^{j-\ell-1}.$$

Proof. This formula is a special case of Theorem 3 in [16], our companion paper with A.S. Lewis, which gives a formula for $\partial f(c, A)$, the Clarke subdifferential[3] [7] of f at (c, A), that applies in both the first and second nonsmooth scenarios discussed above,[4] assuming only that the third does not occur. Under the stronger assumptions made here, $\partial f(c, A)$ consists of only a single point, implying [2, Theorem 6.2.4] that f is differentiable at (c, A), and that its gradient is this point, whose formula is given above.[5] □

[3] The Clarke subdifferential $\partial f(c, A)$ is $\text{conv}\{\lim_{(c^{(k)}, A^{(k)}) \to (c, A)} \nabla f(c^{(k)}, A^{(k)})\}$, where conv denotes convex hull, and the limit is taken over all sequences $((c^{(k)}, A^{(k)}))$ converging to (c, A) on which f is differentiable. As a simple example, the subdifferential of the absolute value function at 0 is the interval $[-1, 1]$, since its gradient is -1 on the negative numbers and 1 on the positive numbers.

[4] In the language of [16], the first case occurs when $Z(c, A)$ contains multiple points, and the second case occurs when $Z(c, A)$ is a singleton but $\Omega(c, A)$ consists of points (ω, v) where there are at least two linearly independent possible choices for v.

[5] Theorem 3 of [16] assumes that the matrix has order greater than one and that the polynomial is not constant, but if $n = 1$, then $W(A)$ consists of a single point, $f(c, A) = 1$ for all (c, A), and it is straightforward to verify that (7) holds with $\nabla f(c, A) = 0$, while if $n > 1$ and $c = [c_0, 0, \ldots, 0]$, representing the constant polynomial $q(c, \zeta) = c_0$, then the assumptions of Theorem 1 do not hold, since if A is not a

4. Smooth stationary points of the Crouzeix ratio

In our optimization experiments, we frequently encounter pairs (c, A) of the following form.

Definition 1. The matrix A has an *outside scalar block* if $A = \mathrm{diag}(\lambda, B)$, $\lambda \in \mathbb{C}$, $\lambda \notin W(B)$. Furthermore, the pair (c, A) has a *dominant* outside scalar block if it also holds that

$$|q(c, \lambda)| > |q(c, \nu)| \text{ for all } \nu \in W(A), \nu \neq \lambda,$$

and

$$|q(c, \lambda)| > \|q(c, B)\|.$$

If A has an outside scalar block then $W(A) = \mathrm{conv}(\lambda, W(B))$ with bd $W(A)$ consisting only of λ, part of bd $W(B)$ and two line segments connecting λ to $W(B)$, as illustrated by the examples reported in Fig. 4 below. Hence, $W(A)$ has a vertex at λ.

Theorem 2. *If (c, A) has a dominant outside scalar block then the Crouzeix ratio f is differentiable at (c, A), its value $f(c, A) = 1$ and its gradient $\nabla f(c, A) = 0$.*

Proof. It is immediate from the assumption that the maximum in the definition of $\tau(c, A)$ is attained only at λ, with $\tau(c, A) = |q(c, \lambda)|$, and that the largest singular value of $q(c, A)$ is simple, with $\beta(c, A) = |q(c, \lambda)|$. Hence $f(c, A) = \tau(c, A)/\beta(c, A) = 1$. Since, for all $\theta \in [0, 2\pi]$, the matrix H_θ has the same block diagonal structure as A, it follows that its normalized eigenvectors have the form either $v = \nu \mathbf{e}_1$, where $\mathbf{e}_1$ is the first coordinate vector and $|\nu| = 1$, and for which $v^* A v = \lambda$, or $v = [0; \tilde{v}]$, for which $\|\tilde{v}\| = 1$ and $v^* A v = \tilde{v}^* B \tilde{v} \in W(B) \not\ni \lambda$. Hence, the only unit vector v for which $v^* A v = \lambda$ is $\mathbf{e}_1$, up to multiplication by a unimodular scalar. We can also take the right singular vector w for the maximum singular value of $q(c, A)$ to be $\mathbf{e}_1$, and then the corresponding left singular vector is $u = \mu \mathbf{e}_1$ where $\mu = q(c, \lambda)/|q(c, \lambda)|$. Since all three assumptions of Theorem 1 are satisfied, f is differentiable at (c, A), with gradient given by (7), with

$$\nabla_c \tau(c, A) = \mu \left[1, \bar{\lambda}, \ldots, \bar{\lambda}^m\right]^T,$$

$$\nabla_A \tau(c, A) = \mu \sum_{j=1}^{m} j \bar{c}_j \bar{\lambda}^{j-1} \mathbf{e}_1 \mathbf{e}_1^T,$$

$$\nabla_c \beta(c, A) = \mu \left[1, \bar{\lambda}, \ldots, \bar{\lambda}^m\right]^T,$$

multiple of the identity matrix the first assumption fails, and if A is a multiple of the identity, the third assumption fails.

$$\nabla_A \beta(c, A) = \mu \sum_{j=1}^{m} \sum_{\ell=0}^{j-1} \bar{c}_j \bar{\lambda}^{\ell} \mathbf{e}_1 \mathbf{e}_1^T \bar{\lambda}^{j-\ell-1}.$$

It follows that $\nabla f(c, A) = 0$. $\square$

Thus, pairs (c, A) which have a dominant outside scalar block, as well as equivalent pairs (c, U^*AU) where U is unitary, are smooth stationary points of the Crouzeix ratio f with stationary value 1. Note that although f is smooth at (c, A), the boundary of the field of values of A is nonsmooth.

If we consider the matrix $\mathrm{diag}(\lambda I, B)$, where I is the identity matrix of order 2 or more, instead of $\mathrm{diag}(\lambda, B)$, we no longer find that the unit vector v for which $v^*Av = \lambda$ is unique up to a scaling, and hence f is not differentiable. Also, if we consider a matrix $A = \mathrm{diag}(\lambda, B)$ with an outside scalar block, where $\tau(c, A)$ is attained at a unique point in the interior of a line segment in bd $W(A)$ instead of the vertex λ, we find, working through the Cowen–Harel parametrization mentioned above, that v is not unique up to a scaling, and hence again f is not differentiable at (c, A).

5. Nonsmooth stationary points of the Crouzeix ratio

Pairs (c, A) for which the Crouzeix ratio is 0.5 are known. Given an integer k with $2 \le k \le \min(n, m+1)$, define the polynomial $p \in \mathcal{P}_m$ by $p(\zeta) = \zeta^{k-1}$, with corresponding coefficient vector

$$c = [c_0, c_1, \ldots, c_{k-1}, \ldots, c_m] = [0, 0, \ldots, 0, 1, 0, \ldots, 0],$$

set the matrix $\Xi_k \in \mathcal{M}^k$ to

$$\begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} \text{ if } k = 2, \text{ or } \begin{bmatrix} 0 & \sqrt{2} & & & & \\ & \cdot & 1 & & & \\ & & \cdot & \cdot & & \\ & & & \cdot & \cdot & \\ & & & & \cdot & 1 \\ & & & & & \cdot & \sqrt{2} \\ & & & & & & 0 \end{bmatrix} \text{ if } k > 2, \tag{8}$$

and set $A = \mathrm{diag}(\Xi_k, 0) \in \mathcal{M}^n$. It was independently observed by Choi [6] and Crouzeix [11] that $W(A) = W(\Xi_k) = \overline{\mathcal{D}}$, so the numerator of the Crouzeix ratio for (c, A) is one, and that $p(A) = A^{k-1} = \mathrm{diag}(\Xi_k^{k-1}, 0)$ is a matrix with just one nonzero, namely a 2 in the $(1, k)$ position, so the denominator of the Crouzeix ratio is 2 and hence the ratio is 0.5. Note that Ξ_k^{k-1} is unitarily similar (via row and column permutations) to a direct sum of a 2×2 Jordan block and a zero matrix of order $k-2$. We call Ξ_k the Choi–Crouzeix matrix of order k.

Since $|p|$ is constant on bd $W(A)$, the Crouzeix ratio f is nonsmooth at (c, A). In [16], together with A.S. Lewis, we showed that $0 \in \partial f(c, A)$, i.e., (c, A) is a nonsmooth stationary point of f. This result extends easily to the pair (c, A) where c is the coefficient vector for $p(\zeta) = (\zeta - \lambda)^{k-1}$ and

$$A = \lambda I + \alpha\, U \mathrm{diag}(\Xi_k, B) U^*, \tag{9}$$

for any nonzero $\alpha, \lambda \in \mathbb{C}$, unitary matrix U, and matrix B with $W(B) \subset \mathcal{D}$. Of course, if Crouzeix's conjecture is true, then these pairs are all global minimizers of f.

Note an interesting difference from the situation in the previous section: here f is nonsmooth at (c, A), although the boundary of the field of values of A is smooth.

6. The computational model

To accurately and efficiently approximate bd $W(A)$, we use Chebfun [13], a system for approximating real- or complex-valued functions to machine precision accuracy by adaptive Chebshev approximation, generating interpolation points z_θ automatically. In the case illustrated in Fig. 1, Chebfun automatically generates a "chebfun" consisting of five "pieces" representing connected sets of extreme points, which must be joined together by line segments to represent all boundary points. The circles plotted in Fig. 1 are in fact the Chebyshev interpolation points z_θ computed by Chebfun.

We have applied two methods for nonsmooth optimization to search for minimizers of the Crouzeix ratio: the Gradient Sampling method [3], which has convergence guarantees described below, and the BFGS method, devised independently in 1970 by Broyden, Fletcher, Goldfarb and Shanno for unconstrained optimization of differentiable functions, but which is also extremely effective for nonsmooth optimization [23], although it does not have convergence guarantees in this domain.

Both the Gradient Sampling method and the BFGS method require computation of $f(c, A)$ and its gradient $\nabla f(c, A)$ at a sequence of iterates $(c^{(k)}, A^{(k)})$ generated by the method. The main cost in computing $f(c, A)$ is that of constructing the chebfun representing bd $W(A)$, including any line segments connecting the extreme points. Computing $\tau(c, A)$, the maximum of the modulus of $q(c, z)$ on bd $W(A)$, is then done by invoking two MATLAB functions that have been overloaded to be applicable to chebfuns, namely `polyval` and `norm(.,inf)`, while computing $\beta(c, A)$, the 2-norm of $q(c, A)$, is carried out by calls to two standard MATLAB functions, `polyvalm` and `norm`.

Once $f(c, A) = \tau(c, A)/\beta(c, A)$ has been computed, the additional computation required to obtain its gradient given by (7) is minimal, even though the formula is somewhat complicated. A natural question is: what is the method to do if f is not differentiable at (c, A)? The answer is that both the Gradient Sampling method and BFGS have the same computational philosophy on this point: there is no need to check whether f is differentiable at (c, A), as the algorithm will virtually never encounter points where f is nonsmooth, except in the limit. In the case of Gradient Sampling this statement can be formalized: convergence results in [21], which refine the original convergence results given by [3], are applicable to the Crouzeix ratio f, since it is locally Lipschitz, continuously differentiable on an open full-measure subset of its domain, and bounded below by zero. Hence, with probability one, Gradient Sampling generates a sequence of points $(c^{(k)}, A^{(k)})$ on which f is differentiable, and for which all cluster points $(\tilde{c}, \tilde{A})$ of the sequence are Clarke stationary, i.e., $0 \in \partial f(\tilde{c}, \tilde{A})$. Thus, the MATLAB codes that compute the Crouzeix ratio can arbitrarily break any ties for the maximum value of $|q(c,z)|$ on bd $W(A)$, ties for the maximum eigenvalue of H_θ, and ties for the maximum singular value of $q(c,A)$, since it is highly unlikely that an exact tie will occur. Clearly, small changes in (c,A) may result in large changes in the computed $\nabla f(c,A)$, but this is inherent in nonsmooth optimization.

The Gradient Sampling and BFGS methods are both line-search descent methods, meaning that at every iteration they use an inexact line search to repeatedly evaluate the minimization objective f along a search direction in the variable space until a reduction in f is obtained.

Gradient Sampling is essentially a stabilized steepest descent method designed for nonsmooth optimization. BFGS is a quasi-Newton method originally designed for smooth optimization problems: the essential idea is that gradient difference information is exploited to update an approximation to the Hessian of the function. In the smooth case, under a regularity condition, eventually the line search takes only unit steps, with just one function evaluation sufficing to obtain a reduction in f, and the asymptotic convergence rate is superlinear. In the nonsmooth case, where the gradient is discontinuous at nonsmooth points, the BFGS update results in a Hessian approximation indicating huge curvature in some directions – exactly what is needed, since a nonsmooth function can always be approximated by a highly ill-conditioned quadratic function. The unit-step and superlinear convergence properties do not hold in the nonsmooth case, but usually not many steps are needed in the line search and the convergence rate is linear. In practice, when BFGS terminates near a point where the function is not differentiable, typically the approximate "Hessian" has condition number of the order of 10^{16}, the inverse of the machine precision, and the algorithm terminates because it cannot obtain descent in the line search due to the limitations of rounding error.

In the next three sections we report results of our experiments that search for a minimizer of the Crouzeix ratio $f(c,A)$ using nonsmooth optimization, along with some theorems and additional conjectures that were inspired by the results. We first treat the case where we vary c and A together; then we describe cases where we fix c and vary A, and finally cases where we fix A and vary c. Since optimizing over complex (c,A) gave similar results to optimizing over real (c,A), but required substantially more time to run, we report only the results for real (c,A), and without loss of generality we optimized over upper Hessenberg matrices A, with all but one subdiagonal set to zero, since any real matrix is orthogonally similar to a Hessenberg matrix and f is invariant under orthogonal similarity transformations. Since $W(A)$ is symmetric w.r.t. the real

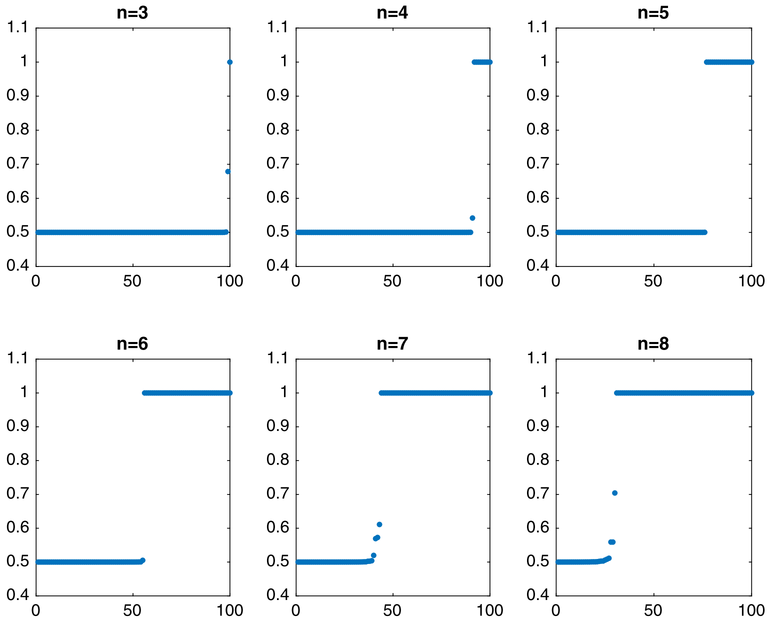

Fig. 2. Results for minimizing f over c and A for $n = 3, \dots, 8$. Each panel shows the final values of f obtained in 100 runs of BFGS from normally distributed starting points, sorted into ascending order.

axis when A is real, we computed bd $W(A)$ only in the upper half plane.[6] Also, since the runs using Gradient Sampling and BFGS gave similar results, but the former required much more computation, we report only the results using BFGS. In each BFGS run, we imposed a maximum of 1000 iterations, stopping earlier if demanding stationarity criteria were met (see [23] for details), or if the method was unable to reduce f in the line search (usually indicating that the current iterate is nearly locally optimal).

The MATLAB codes that we used to generate the results in this paper are available on request to the authors.

7. Varying the polynomial and the matrix

Since Crouzeix's conjecture is known to hold for $n = 2$, we consider $n = 3, \dots, 8$ and, for each n, we set m, the maximum degree of p, to $n - 1$, so that the vector of the corresponding coefficients $c_0, \dots, c_{n-1}$ has length n. Since an $n \times n$ Hessenberg matrix has $(n^2 + 3n - 2)/2$ nonzeros, this amounts to a total of $(n^2 + 5n - 2)/2$ optimization variables. For each n, we made 100 runs of BFGS starting from normally distributed randomly generated starting points. Fig. 2 shows, for each n, the final values of f for each of the 100 starting points, sorted into ascending order. We see that values close

[6] The top half of the boundary is represented by a chebfun parametrized by $\theta \in [\pi, 2\pi]$. In the example of Fig. 1, this chebfun would have 3 smooth pieces, with two line segments connecting them together as well as a third line segment connecting $5 + i$ to the real axis.

Table 1
Results for minimizing f over c and A for $n = 3, \dots, 8$. The second column shows the lowest final value of f over 100 runs of BFGS from normally distributed starting points and the third column shows the eccentricity of the corresponding computed $W(A)$. The next three columns show $|\kappa - \lambda_1|$, $|\kappa - \mu_1|$ and $|\kappa - \mu_2|$ where κ is the center of $W(A)$, λ_1 is the smallest root (in magnitude) of p and μ_1, μ_2 are the two eigenvalues of A that are closest to κ, with p and A respectively the polynomial corresponding to the final coefficient vector c and the final matrix. The meaning of the final two columns is explained in the text.

n	f	ecc($W(A)$)	$\lvert\kappa - \lambda_1\rvert$	$\lvert\kappa - \mu_1\rvert$	$\lvert\kappa - \mu_2\rvert$	$\lVert d\rVert$	$\lVert E\rVert$
3	0.500000000000000	2.1e−08	1.2e−11	2.2e−07	2.2e−07	3.3e−12	3.1e−05
4	0.500000000000000	1.9e−04	1.2e−08	1.7e−04	1.7e−04	3.3e−08	1.9e−06
5	0.500000000000014	3.2e−04	2.6e−08	5.0e−04	5.0e−04	1.7e−08	1.3e−04
6	0.500000017156953	8.4e−02	3.5e−01	1.7e−01	3.2e−01	4.4e+00	NaN
7	0.500000746246673	1.2e−01	1.6e−01	4.4e−01	1.0e+00	5.7e+00	NaN
8	0.500000206563813	1.3e−01	5.1e−01	7.2e−01	7.5e−01	8.8e+00	NaN

to 0.5 are found repeatedly, for all $n = 3, \dots, 8$, and no lower values were found. (We will discuss the values near 1 below.) The fact that the minimal value found is so often close to 0.5 is strong evidence that 0.5 is at least a *locally* minimal value for f; it also indicates substantial support for the conjecture that this is the *globally* minimal value. Examining the second column of Table 1, we see that, for each n, the lowest value of f found approximates 0.5 quite accurately, ranging from 15 decimal digits of agreement for $n = 3$ (about the best that is possible using IEEE double precision in MATLAB) to 6 digits for $n = 8$.

Fig. 3 shows, for each n, the boundary of the field of values of A, the eigenvalues of A, and the roots of p, where A and p are respectively the final computed matrix and polynomial (with coefficients given by c) associated with the lowest final Crouzeix ratio f. In all cases, $W(A)$ is close to a disk, as further verified by the eccentricities[7] reported in the third column of Table 1, but there are some subtle distinctions between the results for the various values of n.

In the panels for $n = 3$, 4 and 5, for which the final value of f approximates 0.5 to between 13 and 15 digits, we see that exactly *one* root of p, denoted λ_1, and *two* eigenvalues of A, denoted μ_1 and μ_2, are very nearly coincident with κ, the center[8] of $W(A)$; their distances from κ are displayed in Table 1. Define the coefficient vectors

$$\tilde{c} = \frac{1}{c_1} c \text{ and } d = \frac{1}{c_1}[0, 0, c_2, \dots, c_{n-1}], \text{ so that } \tilde{c} - d = \left[\frac{c_0}{c_1}, 1, 0, \dots, 0\right].$$

The penultimate column of Table 1 displays the norm of d, which measures how close $\tilde{c}$ is to being a linear polynomial. When $\|d\|$ is small, as it is for $n = 3$, 4 and 5, all the roots of p except $\lambda_1 \approx -c_0/c_1$ are enormous (they diverge to ∞ as the coefficients

[7] Defined as $(1 - b^2/a^2)^{1/2}$, where a and b are respectively the maximum and minimum of the real and imaginary diameters of $W(A)$, giving zero if $W(A)$ is a disk.

[8] Computed as the real part of the integral of the chebfun representing bd $W(A)$ in the upper half-plane, divided by π.

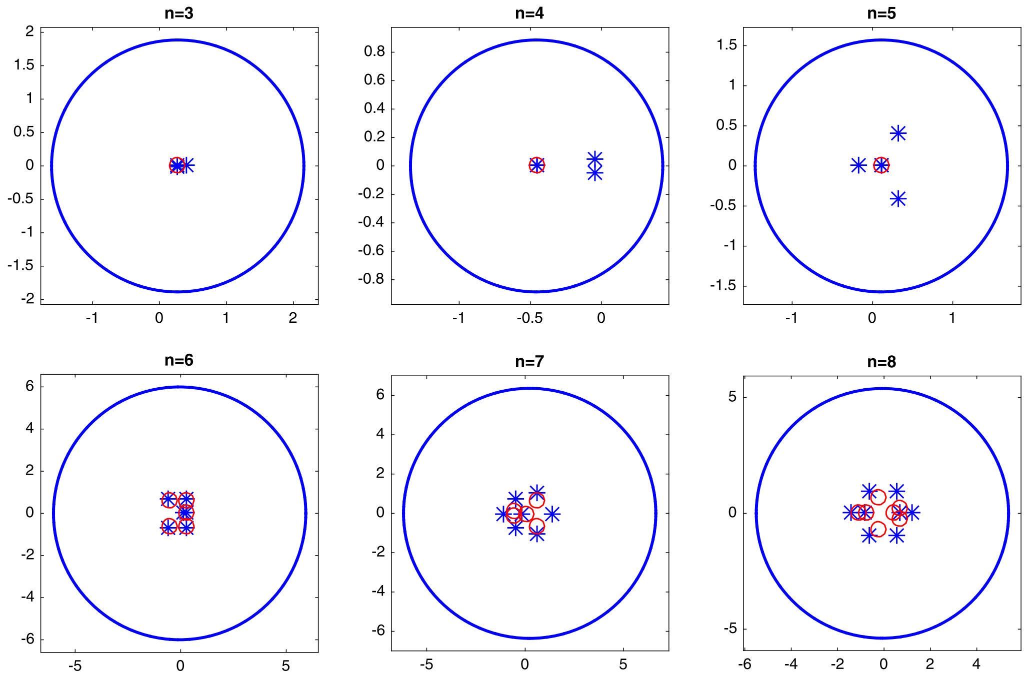

Fig. 3. Results for minimizing f over c and A for $n = 3, \ldots, 8$. The panel for each n shows the boundary of $W(A)$ (solid curve), the eigenvalues of A (asterisks) and the roots of p (small circles), where p and A are respectively the final polynomial and matrix corresponding to the lowest final value of f, all plotted in the complex plane. Roots of p lying outside $W(A)$ are not shown.

$c_2, \ldots, c_{n-1}$ converge to zero). Furthermore, we find using the Generalized Null Space Decomposition (GNSD)[9] that

$$A - \lambda I = \alpha\, U \mathrm{diag}(\Xi, B) U^T + E, \tag{10}$$

where $\lambda = \lambda_1$, $0.5 < \alpha < 4$, U is orthogonal, $\Xi = \Xi_2$ (the 2×2 Choi–Crouzeix matrix given in (8)), $W(B) \subset \mathcal{D}$ and $\|E\|$ is given in the last column of Table 1. Since, for $n = 3$, 4 and 5, $\|d\|$ and $\|E\|$ are both small, the pair $(\tilde{c}, A)$ is close to a pair $(\tilde{c} - d, A - E)$ which is *precisely* a nonsmooth stationary point of the kind discussed in Section 5, with $k = 2$.

Although most of the final pairs (c, A) for which f agrees with 0.5 to about 15 digits have the configuration just described, some have roots $\lambda_1, \ldots, \lambda_{k-1}$ of p and eigenvalues $\mu_1, \ldots, \mu_k$ of A nearly coincident for $k > 2$, with coefficients $c_k, \ldots, c_{n-1}$ close to zero and with (10) holding as above, except that $\lambda = (\sum_{j=1}^{k-1} \lambda_j)/(k-1)$, Ξ is the $k \times k$ Choi–Crouzeix matrix given in (8) with $k > 2$, and $\|B^{k-1}\| < 2$. These pairs (c, A) are also close to being nonsmooth stationary points of the kind discussed in Section 5.

9 See [17] for the history of the GNSD, more often known as the staircase form, which goes back to [22]. We used the MATLAB code available in the supplementary online materials published with [17]. This requires an input tolerance, but the results given here are identical for tolerances in the range 10^{-6} to 10^{-1}.

The results for $n = 6$, 7, and 8 are quite different. The final polynomial p does not have any small coefficients, and hence does not have any huge roots. Instead, all roots of p as well as all eigenvalues of A are approximately near κ, the center of $W(A)$, but none of them is nearly coincident with κ or with any of the other roots or eigenvalues. Furthermore, as can be seen from the eccentricities, $W(A)$ is not as close to being a disk as it is in the cases $n = 3$, 4 and 5. We have observed repeatedly that this kind of configuration, with the roots of p and the eigenvalues of A all clustered fairly near, but not very near, the center of an approximate disk $W(A)$, is typical for approximate minimizers of the Crouzeix ratio with values fairly, but not very, close to 0.5.

Another striking observation from Fig. 2 is that the final value of f equals 1 for a significant number of starting points, ranging from just 1% for $n = 3$ to 70% for $n = 8$. The corresponding final computed (c, A) all have the property that[10]

$$A = U\mathrm{diag}(\lambda, B)U^T + E$$

where $(c, \mathrm{diag}(\lambda, B))$ has a dominant outside scalar block λ (see Definition 1), U is orthogonal and $\|E\|$ is small, typically of the order of 10^{-8}. Hence, according to Theorem 2, the pairs $(c, A - E)$ are smooth stationary points of f. Further numerical investigation indicates that they are local minimizers, as is also indicated by the fact that we repeatedly find these stationary values. Fig. 4 shows, for $n = 3, \ldots, 8$, the fields of values for which f is closest to 1 — in fact, agreeing with the value 1 to 15 digits. Note the "ice cream cone" shapes of these fields of values, with the dominant scalar block λ at the vertex. As n is increased, it becomes increasing difficult for BFGS from randomly generated starting points to find any values of f below 1.

There are a few final computed values of f displayed in Fig. 2 that are not close to 0.5 or 1, so we restarted BFGS at the corresponding final pairs (c, A) and at nearby points using various perturbation levels. For $n = 3$ and 4, we quickly found values of f that were close to 0.5. For $n = 5$ and 6, there were no final values that were not close to 0.5 or 1, so no restarts were needed. However, for $n = 7$ and 8, restarting BFGS at and near the final computed pairs did not lead to much improvement, suggesting the possibility that there are other stationary values of f between 0.5 and 1.

8. Fixing the polynomial, varying the matrix

Additional insight is gained by fixing $p \in \mathcal{P}_m$, allowing A to vary over $n \times n$ matrices. The case $p(\zeta) = \zeta^m$ is addressed first. In this case, as mentioned in Section 1, we know that Crouzeix's conjecture holds, so finding values of f lower than 0.5 is impossible. The interest in these experiments is in discovering for what A we find f equal to or close to 0.5. The results are completely different for the cases $n > m$ and $n \leq m$.

[10] Computed from the Schur decomposition of A, permuting the eigenvalues if necessary to ensure that the dominant one appears in the 1,1 position. This can be done in MATLAB using the `ordschur` function.

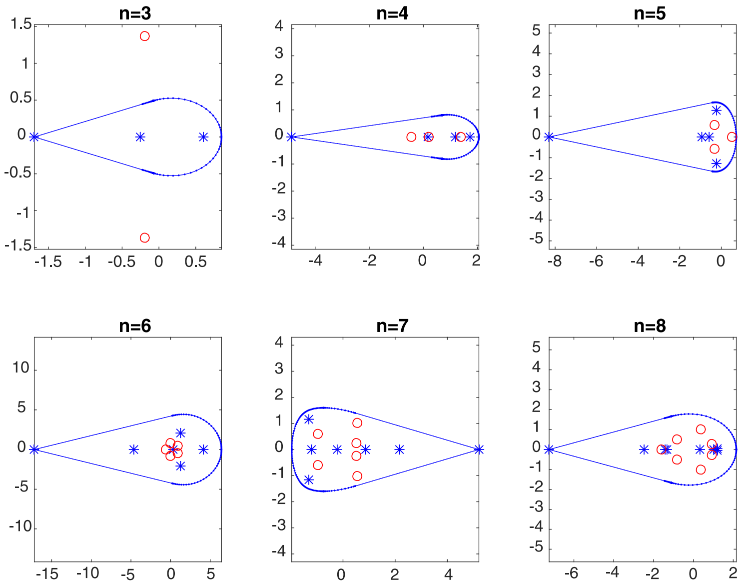

Fig. 4. "Ice Cream Cone" stationary points of the Crouzeix ratio f, discovered while minimizing f for $n = 3, \ldots, 8$. The panel for each n shows the boundary of $W(A)$ (solid curve), the eigenvalues of A (asterisks) and the roots of p (small circles), where p and A are respectively the final polynomial and matrix corresponding to the final value of f that is *closest to one*, all plotted in the complex plane.

8.1. When $p(\zeta) = \zeta^m$ and $n > m$

As in the previous section, we optimized the Crouzeix ratio f over $n \times n$ real upper Hessenberg matrices, with n ranging from 3 to 8, but this time with p fixed to the monomial $p(\zeta) = \zeta^m$, with $m = n - 1$, so $c = [0, \ldots, 0, 1]$. Fig. 5 displays the final values of f, again starting BFGS from 100 randomly generated starting points, sorted into ascending order. As before, many values close to 0.5 or equal to 1 were found, but other apparently locally minimal values between 0.5 and 1 were also discovered, for $n = 4, \ldots, 8$. Fig. 6 shows, for each n, the boundary of $W(A)$ where A is the final matrix associated with the lowest value of f, along with the eigenvalues of A and the single root 0 of p. The fields of values of the final matrices are somewhat closer to being disks than previously, as the eccentricities shown in Table 2 are now smaller. The table also shows the smallest and largest eigenvalues of A in modulus. The most important difference from the results of the previous section is that for $n = 3$, 4, 5 and 6, *all* n eigenvalues of A are close to zero, and (10) now holds with $\lambda = 0$, $\|E\|$ small and $\Xi = \Xi_n$, the $n \times n$ Choi–Crouzeix matrix given in (8).

Based on these results and others, we conjecture that, when $p(\zeta) = \zeta^{n-1}$, with corresponding coefficient vector c, the *only* $n \times n$ matrices A for which $f(c, A) = 0.5$ are those of the form $\alpha\, U \Xi_n U^*$, where $\alpha \neq 0$ and U is unitary, and for $p(\zeta) = \zeta^m$ and A of order $n > m$, a matrix of the form $\alpha\, U \mathrm{diag}(\Xi_{m+1}, B) U^*$, where $\alpha \neq 0$, U is unitary and $W(B) \subseteq \overline{\mathcal{D}}$.

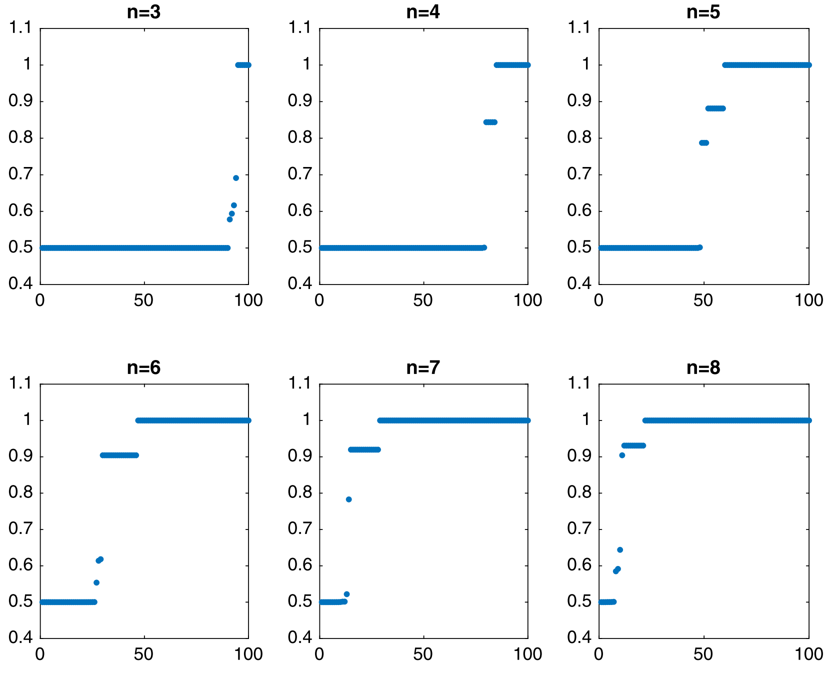

Fig. 5. Results for minimizing f over A for $n = 3, \ldots, 8$, with p fixed to the monomial ζ^{n-1}. Each panel shows the final values of f obtained in 100 runs of BFGS from normally distributed starting points, sorted into ascending order.

Table 2
Results for minimizing f over A for $n = 3, \ldots, 8$, with p fixed to the monomial ζ^{n-1}. The second column shows the lowest final value of f over 100 runs of BFGS from normally distributed starting points and the third column shows the eccentricity of the corresponding computed $W(A)$. The remaining columns show $|\kappa|$, $|\mu_1|$ and $|\mu_n|$ where κ is the center of $W(A)$, and μ_1 and μ_n are respectively the smallest and largest eigenvalues of A in modulus, where A is the matrix associated with the lowest value of f.

n	f	ecc($W(A)$)	$\|\kappa\|$	$\|\mu_1\|$	$\|\mu_n\|$	$\|E\|$
3	0.500000000000000	0.0e+00	1.5e−16	1.3e−05	1.3e−05	1.9e−08
4	0.500000000000000	1.5e−08	3.4e−16	6.8e−04	6.8e−04	1.5e−07
5	0.500000000000002	2.1e−08	3.1e−16	1.3e−03	3.9e−03	1.8e−07
6	0.500000000000129	1.9e−07	8.8e−16	1.9e−03	7.4e−02	2.6e−06
7	0.500002622037000	9.2e−04	1.6e−06	7.0e−01	1.7e+00	NaN
8	0.500040868776241	2.7e−03	8.7e−06	1.2e+00	2.9e+00	NaN

8.2. When $p(\zeta) = \zeta^m$ and $n \le m$

When we fix p to the monomial ζ^m but insist that the matrix A have order $n \le m$, we are no longer able to find values of the Crouzeix ratio f that are close to 0.5, as illustrated in Fig. 7 in the case $n = m$. We conjecture that when $p(\zeta) = \zeta^m$ there is no sequence of matrices of order $n \le m$ for which the Crouzeix ratio converges to 0.5. Note that $\Xi_n^n = 0$, so for A close to Ξ_n the Crouzeix ratio is large.

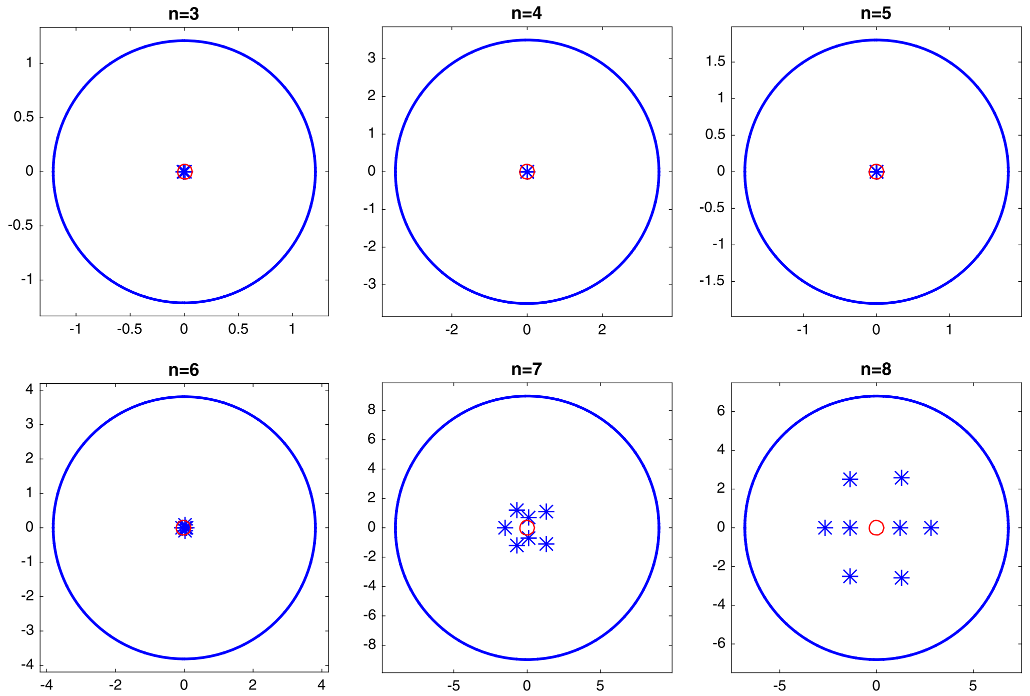

Fig. 6. Results for minimizing f over A for $n = 3, \ldots, 8$, with p fixed to the monomial ζ^{n-1}. The panel for each n shows the boundary of $W(A)$ (solid curve), the eigenvalues of A (asterisks) and the origin (small circle), where A is the matrix corresponding to the lowest final value of f.

8.3. When p is arbitrary and $n > m$

When we fix p to be any polynomial of degree m *except* a monomial, and we optimize over $(m+1) \times (m+1)$ matrices, we are able to generate values of the Crouzeix ratio that approximate 0.5, but the closer we approximate it, the larger $W(A)$ becomes, so that the limit 0.5 is not actually attained. This observation led us to the following theorem.

Theorem 3. *For any fixed polynomial p of degree $m \geq 1$, with corresponding coefficient vector c, there exists a divergent sequence $\{A^{(k)}\}$ of order $n = m + 1$ for which $f(c, A^{(k)})$ converges to 0.5. Furthermore, we can choose the sequence so that $\{W(A^{(k)})\}$ are disks.*

Proof. Let $A^{(k)} = k\,\Xi_{m+1}$, where Ξ_{m+1} is the Choi–Crouzeix matrix given in (8). Then $W(A^{(k)})$ is a disk centered at 0 with radius k. Write $p(\zeta) = c_m\zeta^m + \cdots + c_0$. Then the $(1, n)$ entry of $p(A^{(k)})$ is $2c_m k^m$, so $2|c_m|k^m$ dominates $\|p(A^{(k)})\|$ as $k \to \infty$. Furthermore, $\|p\|_{W(A^{(k)})}$ is increasingly well approximated by $|c_m|k^m$ as $k \to \infty$. So, $f(c, A^{(k)}) \to 0.5$ as $k \to \infty$. $\square$

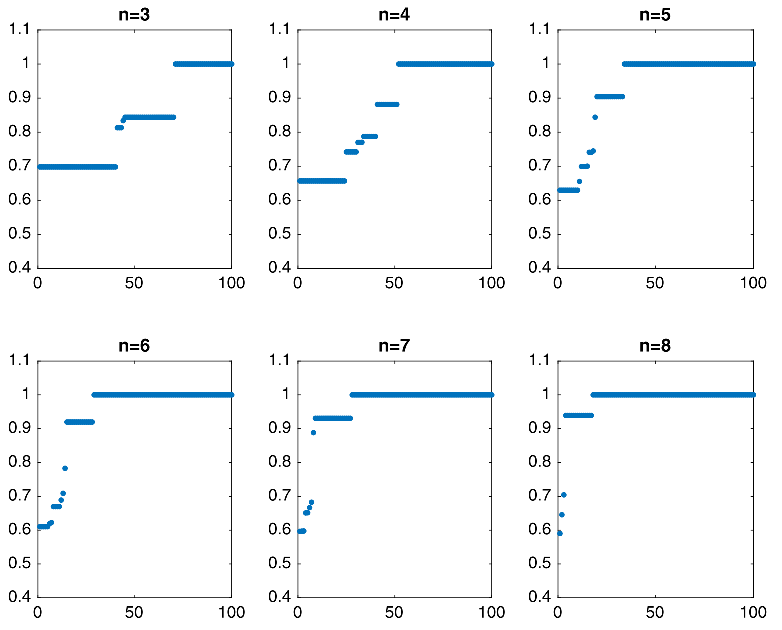

Fig. 7. Results for minimizing f over A for $n = 3, \ldots, 8$, with p fixed to the monomial ζ^n. Each panel shows the final values of f obtained in 100 runs of BFGS from normally distributed starting points, sorted into ascending order.

Note also that if $p(\zeta) = \zeta^m$, then $f(c, A^{(k)}) = 0.5$ for all k, so there is no need for $W(A)$ to blow up in this case and we can replace the sequence $\{A^{(k)}\}$ by the constant matrix Ξ_{m+1}.

We conjecture that when p is fixed to be any polynomial of fixed degree m *except* a monomial, with corresponding coefficient vector c, it is not possible to find A with order $m + 1$, or indeed any larger order, for which $f(c, A) = 0.5$. However, 0.5 can be approximated to arbitrary accuracy by blowing up $W(A)$ sufficiently, and attained when p is a monomial, as explained above.

8.4. When p is arbitrary and $n \le m$

When we fix p with degree m with at least two distinct roots and optimize over A with size $n = m$, we find very different behavior. We frequently generate a sequence of matrices for which $W(A)$ shrinks to a single point, namely, one of the roots of p, with f converging to 0.5, but as in the previous subsection, the limit 0.5 is not actually attained. This observation led us to the following theorem.

Theorem 4. *Fix p to have degree m with at least two distinct roots and with corresponding coefficient vector c. Then, for all integers n with $2 \le n \le m$, there exists a convergent sequence of $n \times n$ matrices $\{A^{(k)}\}$ for which the Crouzeix ratio $f(c, A^{(k)})$ converges to* 0.5.

Furthermore, we can choose $A^{(k)}$ so $\{W(A^{(k)})\}$ is a sequence of disks shrinking to a root of p.

Proof. Without loss of generality we can assume that one of the roots of p is zero, so

$$p(\zeta) = \zeta^\ell \prod_{i=1}^{m-\ell} (\lambda_i - \zeta)$$

where ℓ is the multiplicity of the zero root, and the other roots λ_i, $i = 1, \ldots, m - \ell$, are nonzero, though not necessarily distinct from each other. Let $A^{(k)}$ be zero except that its leading $(\ell + 1) \times (\ell + 1)$ submatrix is $\Xi_{\ell+1}/k$. Then

$$p(A^{(k)}) = (A^{(k)})^\ell \prod_{i=1}^{m-\ell} (\lambda_i I - A^{(k)})$$

is a matrix that is all zero except that its $(1, \ell + 1)$ entry is $2(1/k)^\ell \prod_{i=1}^{m-\ell} \lambda_i$, so $\|p(A^{(k)})\| = 2(1/k)^\ell \prod_{i=1}^{m-\ell} |\lambda_i|$. Furthermore, $W(A^{(k)})$ is a disk around 0 of radius $1/k$, so for large k the maximum of $|p(\zeta)|$ on this disk is increasingly well approximated by $(1/k)^\ell \prod_{i=1}^{m-\ell} |\lambda_i|$. Hence, $f(c, A^{(k)}) \to 0.5$ as $k \to \infty$. $\square$

Note that the quantity 0.5 is not attained as in the limit one instead obtains 0/0.

We conjecture that when p is fixed to be *any* polynomial of fixed degree m, with corresponding coefficient vector c, it is not possible to find A with order m, or less, for which $f(c, A) = 0.5$. However, as long as p has at least two distinct roots, 0.5 can be approximated to any accuracy by shrinking $W(A)$ sufficiently close to one of the roots, as explained above.

9. Fixing the matrix, varying the polynomial

If we fix A, then in general the Crouzeix ratio 0.5 cannot be attained or approximated to arbitrary accuracy by some p of fixed maximal degree. Obviously this is true if A is normal, but we conjecture that it is true for all A unless it is essentially a Choi–Crouzeix matrix, that is a matrix of the form (9).[11]

Suppose we remove the limitation on the maximum degree of p. It is known that for any fixed A, any analytic function g that minimizes $\|g\|_{W(A)}/\|g(A)\|$ has constant magnitude on bd $W(A)$ [8], and it is possible to compute this numerically using conformal mapping techniques and Blaschke products. This work is beyond the scope of the paper, so we leave discussion of this to future work.

[11] Extended to allow $W(B) \subseteq \overline{\mathcal{D}}$: this possibility is not included in (9) as the variational analysis result does not extend to this case.

10. Summary

In this paper, we investigated Crouzeix's conjecture by optimizing the Crouzeix ratio f defined in (5), whose minimum value over all polynomials p and matrices A is 0.5 if the conjecture is true. We used Chebfun to approximate the boundary of the field of values $W(A)$ to high accuracy and BFGS to search for minimizers of f over the variable space (c, A), where c is the coefficient vector for the polynomial p. It is remarkable how reliably Chebfun and BFGS performed despite the nonsmoothness that can occur either in the boundary of $W(A)$ (w.r.t. the complex plane) or in the Crouzeix ratio f (w.r.t. the variable space). The results for the 600 runs of BFGS reported in Fig. 2 alone required about 500,000 chebfun constructions, each one to represent the field of values of a different matrix, including all the evaluations of $f(c, A)$ carried out in the line searches. Almost all these runs delivered pairs (c, A) that are either (i) close to a nonsmooth stationary point of f with stationary value 0.5 (for which p is a monomial with degree m and A is essentially[12] a Choi–Crouzeix matrix of order $m+1$, with $W(A)$ being a disk) or (ii) close to a smooth stationary point of f with stationary value 1 (for which (c, A) has a dominant outside scalar block, with $W(A)$ having an "ice-cream-cone" shape).

We also searched for minimizers of the Crouzeix ratio when the polynomial is fixed. The resulting observations led to Theorems 3 and 4, which show that given any fixed polynomial with at least two distinct roots, there is a sequence of matrices of any given order on which the Crouzeix ratio converges to 0.5.

Overall, our results strongly support Crouzeix's conjecture: the globally minimal value of f is 0.5.

Acknowledgements

We especially thank Nick Trefethen for suggesting investigation of Crouzeix's conjecture using Chebfun and for his interest in this work. Thanks also to Nick Hale and Anthony Austin for their invaluable help responding to our questions about Chebfun and providing support when it was needed. We also warmly thank Michel Crouzeix for many interesting discussions, both by email and in person.

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[12] More precisely, has the form (9), with $k = m + 1$.

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