CONDITION ESTIMATES FOR PSEUDO-ARCLENGTH CONTINUATION *

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Abstract. We bound the condition number of the Jacobian in pseudo arclength continuation problems, and we quantify the effect of this condition number on the linear system solution in a Newton GMRES solve.

In pseudo arclength continuation one repeatedly solves systems of nonlinear equations $F(u(s), \lambda(s)) = 0$ for a real-valued function u and a real parameter λ, given different values of the arclength s. It is known that the Jacobian F_x of F with respect to $x = (u, \lambda)$ is nonsingular, if the path contains only regular points and simple fold singularities. We introduce a new characterization of simple folds in terms of the singular value decomposition, and we use it to derive a new bound for the norm of F_x^{-1}. We also show that the convergence rate of GMRES in a Newton step for $F(u(s), \lambda(s)) = 0$ is essentially the same as that of the original problem $G(u, \lambda) = 0$. In particular we prove that the bounds on the degrees of the minimal polynomials of the Jacobians F_x and G_u differ by at most 2. We illustrate the effectiveness of our bounds with an example from radiative transfer theory.

Key words. Pseudo-Arclength Continuation, singularity, GMRES, singular vectors, eigenvalues, rank-one update

AMS subject classifications. 65H10, 65H17, 65H20, 65F10, 65F15

1. Introduction. Numerical continuation is the process of solving systems of nonlinear equations $G(u, \lambda) = 0$ for various values of a real parameter λ. Here $u : R^N \to R$ is a real-valued function and $G : R^{N+1} \to R^N$. An obvious approach for implementing numerical continuation, called *parameter continuation* [6,9,15], traces out a solution path by repeatedly incrementing λ until the desired value of λ is reached. In each such iteration, the current solution u is used as an initial iterate for the next value of λ. Although parameter continuation is simple and intuitive, it fails at points (u, λ) where the Jacobian G_u is singular. In this paper we consider singularities which are simple folds.

The standard way to remedy the failure of parameter continuation at simple folds is to reparameterize the problem by introducing the arclength parameter, s, so that both u and λ depend on s. This idea, known as *pseudo-arclength continuation* [6,9,15], implements parameter continuation on $F(u(s), \lambda(s)) = 0$ with s as the parameter instead of solving $G(u, \lambda) = 0$ with λ as the parameter. Thus pseudo-arclength continuation requires that the Jacobian F_x of F be nonsingular. It is known that F_x is nonsingular at simple folds and points where G_u is nonsingular [9].

Our first goal (§ 3) is to quantify this nonsingularity. To this end we provide a new characterization of simple folds in terms of the singular value decomposition (SVD) of G_u. From the SVD, we derive a new bound for $\|F_x^{-1}\|_2$. This bound can be used to limit the

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arclength step in Newton's method. As a byproduct we obtain a refinement of Weyl's monotonicity theorem [19] for the smallest eigenvalue of a symmetric positive semi-definite matrix (§3.1).

We also examine (§4) how the conditioning of F_x affects the convergence of the inner GMRES [20] iteration in a Newton-GMRES solver [1,2,11,12]. We show that the eigenvalue clustering of the Jacobian F_x in the reformulated problem is not much different from that of the Jacobian G_u in the original problem. To be precise, the upper bound on the degree of the minimal polynomial of F_x differs from that of G_u by at most two. This implies [3,14] that the convergence of GMRES as a linear solver in a Newton step does not slow down when parameter continuation is replaced by pseudo-arclength continuation.

At last (§5) we illustrate our findings with a numerical example from radiative transfer theory. These numerical results, combined with our bounds, support the use of pseudo-arclength continuation in solution paths that contain simple folds.

2. Background. We briefly review theory and algorithms for solving numerical continuation problems $G(u,\lambda) = 0$, where $\lambda \in R$, $u : R^N \to R$ and $G : R^{N+1} \to R^N$. We discuss parameter continuation §2.1 and pseudo-arclength continuation in §2.2. We use the abbreviations

$$G_u \equiv \frac{\partial G}{\partial u}, \qquad G_\lambda \equiv \frac{\partial G}{\partial \lambda}.$$

2.1. Simple parameter continuation. Parameter continuation [6,9,15] is the simplest method for solving $G(u,\lambda) = 0$. The idea is to start at a point $\lambda = \lambda_{init}$ and solve $G(u,\lambda)$ for u, say by Newton's method. Use the solution u_0 as the initial iterate to solve the next problem $G(u, \lambda + d\lambda) = 0$. Algorithm `paramc` below is a simple implementation of parameter continuation from λ_{init} to $\lambda_{end} = \lambda_{init} + n\, d\lambda$ where n denotes the maximum number of continuation iterations.

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paramc$(u, G, \lambda_{init}, \lambda_{end}, d\lambda)$
  Set $\lambda = \lambda_{init}$, $u_0 = u$
  while $\lambda \leq \lambda_{end}$ **do**
    Solve $G(u,\lambda) = 0$ with u_0 as the initial iterate to obtain u_1
    $u_0 = u_1$
    $\lambda = \lambda + d\lambda$
  end while

While parameter continuation appears to be a reasonable method for solving $G(u,\lambda) = 0$, it fails at points that violate the assumptions of the implicit function theorem. Such points of failure are called singular points.

DEFINITION 2.1. *A* **singular point** *is a solution* (u_0, λ_0) *to* $G(u,\lambda) = 0$ *for which* $G_u(u_0, \lambda_0)$ *is singular.*

In order to understand why parameter continuation fails at singular points, we recall the implicit function theorem [9, 18]. The norm $\|\cdot\|$ denotes the Euclidean norm, and

$C^k(\Omega)$ denotes the space of k times continuously differentiable functions from an open subset $\Omega \subset R^{N+1}$ to R^N.

THEOREM 2.2. *[**Implicit Function Theorem:**] Let Ω be an open subset of R^{N+1} and let $G \in C^k(\Omega)$ for some integer $k > 0$. Let G_u and G_λ be Lipschitz continuous in $\bar{\Omega}$, the closure of Ω. If*

- $(u_0, \lambda_0) \in \Omega$,
- $G(u_0, \lambda_0) = 0$,
- $G_u(u_0, \lambda_0)$ *is nonsingular,*

then there are $\rho > 0$ and $\epsilon > 0$ such that there is a unique solution

$$v \in \mathcal{B}_\rho(u_0) \equiv \{u \,|\, \|u - u_0\| < \rho\}$$

of $G(u, \lambda) = 0$ for all $\lambda \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon)$ and $u \in \mathcal{B}_\rho(u_0)$. Furthermore, v is a k times continuously differentiable function of λ.

If the assumptions of the implicit function theorem are satisfied then Newton's method converges q-quadratically, as shown below. We will use the following definition of quadratic convergence for Newton's method.

DEFINITION 2.3. *Let $\{x_n\} \subset R^N$ be a sequence and let $x^* \in R^N$. We say that $x_n \to x^*$* **q-quadratically** *as $n \to \infty$, if $x_n \to x^*$ and if there is $K > 0$ such that*

$$\|x_{n+1} - x^*\| \leq K\|x_n - x^*\|^2.$$

The following corollary presents conditions under which Newton's method applied to $G(u, \lambda) = 0$ converges q-quadratically.

COROLLARY 2.4. *Let the assumptions of Theorem 2.2 hold. Then there is $\delta > 0$, which depends only on $\|G_u^{-1}(u_0, \lambda_0)\|$ and the Lipschitz constants of G_u and u, such that if $|\lambda - \lambda_0| < \delta$ then Newton's method with initial iterate u_0 converges q-quadratically to the solution u^*.*

Proof. Define the Lipschitz constants

$$\|u(\lambda) - u(\mu)\| \leq \gamma_u|\lambda - \mu|, \qquad \|G_u(u, \lambda) - G_u(v, \mu)\| \leq \gamma_G(\|u - v\|| + |\lambda - \mu|).$$

According to [11]

$$\|u_0 - u^*\| < \frac{1}{2\gamma_G\|G_u^{-1}(u_0, \lambda_0)\|}$$

so choosing

$$\delta < \frac{1}{2\gamma_u\gamma_G\|G_u^{-1}(u_0, \lambda_0)\|}$$

completes the proof. □

Theorem 2.2 and Corollary 2.4 suggest that points (u, λ) for which G_u is singular may cause the loss of uniqueness in the solution to $G(u, \lambda) = 0$ as well as the failure of Newton's method, and therefore failure of Algorithm `paramc`. Thus we need a continuation method that does not fail at singular points.

2.2. Pseudo-arclength Continuation. Pseudo-arclength continuation [6,9,15] avoids the problems of Algorithm `paramc` at singular points by using an arclength parameterization. The curve in Figure 5.1, for instance, has a singularity with respect to the parameter λ. If we choose arclength s as the parameter λ, and $x = (u^T, \lambda)^T$ in place of u, we can compute the curve with simple parameter continuation. The curve in Figure 5.1 has a simple fold, which is the singularity of interest for this paper. Formally, a simple fold is defined as follows.

DEFINITION 2.5. *A solution* (u_0, λ_0) *of* $G(u, \lambda) = 0$ *is a* **simple fold** *if*
- $dim(Ker(G_u(u_0, \lambda_0))) = 1$ *and*
- $G_\lambda(u_0, \lambda_0) \notin Range(G_u(u_0, \lambda_0))$.

To develop a pseudo-arclength continuation method, we assume that x depends smoothly on s. Then one can differentiate $G(u, \lambda) = 0$ with respect to s and obtain

$$\frac{dG(u(s), \lambda(s))}{ds} = G_u \dot{u} + G_\lambda \dot{\lambda} = 0. \tag{2.1}$$

Equivalently, one can differentiate $G(x) = 0$ and obtain $G_x \dot{x} = 0$. Here, $\dot{x}$ denotes the derivative with respect to s. Because the norm is the Euclidean norm and s is arclength,

$$\|\dot{x}\|^2 = \|\dot{u}\|^2 + |\dot{\lambda}|^2 = 1. \tag{2.2}$$

Since we introduced a new parameter s, we must add an equation to $G(u, \lambda) = 0$ so that the number of equations equals the number of unknowns and we have a chance of obtaining a nonsingular Jacobian for the reformulated problem. Hence, we work with the extended equations

$$F(x, s) = \begin{pmatrix} G(x) \\ \mathcal{N}(x, s) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{2.3}$$

The normalization equation $\mathcal{N} = 0$ is an approximation of (2.2) where

$$\mathcal{N}(x, s) = \dot{x}_0^T (x - x_0) - (s - s_0) = 0. \tag{2.4}$$

This equation says that the new point on the path lies on the tangent vector through the current point x_0.

Given a known point (x_0, s_0), the pseudo-arclength continuation method increments arclength by $ds = s - s_0$, and solves (2.3) with the normalization (2.4) by Newton's method with initial iterate x_0. Algorithm `psarc` is a simple implementation of pseudo-arclength continuation.

Since pseudo-arclength continuation is just simple parameter continuation applied to F with s as the parameter, Corollary 2.4 gives conditions for the convergence of Newton's method in pseudo-arclength continuation.

COROLLARY 2.6. *Let the assumptions of Theorem 2.2 hold for* F. *Then there is* $\delta > 0$, *which depends only on* $\|F_x^{-1}(x_0, s_0)\|$ *and the Lipschitz constants of* F_x *and* x, *such that if* $|s - s_0| < \delta$ *then Newton's method with initial iterate* x_0 *converges q-quadratically to the solution.*

psarc$(u, F, s_{end}, d\lambda)$
  Set $s = 0$, $x_0 = (u_0^T, \lambda_0)^T$
  while $s \leq s_{end}$ **do**
    Approximate $\dot{x}$
    Solve $F(x, s) = 0$ with x_0 as the initial iterate obtain x_1
    $x_0 = x_1$
    $s = s + ds$
  end while

The proof of Corollary 2.4 shows that the step in arclength is bounded by

$$\delta < \frac{1}{2\gamma_x \gamma_F \|F_x^{-1}(x_0, s_0)\|},$$

where γ_x and γ_F are Lipschitz constants for x and F, respectively. Therefore a bound on $\|F_x^{-1}\|$ is an important factor in bounding the arclength step. In the next section we present the main result of this paper, a new bound on $\|F_x^{-1}\|$.

3. Nonsingularity of F_x. For a solution $x_0 = (u_0, \lambda_0)$ to $G(u, \lambda) = 0$, we present an upper bound on $\|F_x^{-1}(x_0, s_0)\|$ in the case that

- $G_u(u_0, \lambda_0)$ is nonsingular or
- (u_0, λ_0) is a simple fold of $G(u, \lambda) = 0$.

In order to derive the bound, we introduce a new characterization of simple fold, which is based on the singular value decomposition of G_u. We prove the bound in §3.2. In §3.1 we refine Weyl's monotonicity theorem for the smallest eigenvalue of a symmetric positive semi-definite matrix, which we need for the proof.

Let

$$G_u(u, \lambda) = U \Sigma V^T$$

be a singular value decomposition (SVD) of $G_u(u, \lambda)$ where

$$\Sigma = diag(\sigma_1, \sigma_2, \ldots, \sigma_N), \qquad \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_N \quad and \qquad u_N \equiv U e_N$$

where e_N is the last column of the $N \times N$ identity matrix. The trailing column u_N of U is a left singular vector associated with the smallest singular value σ_N. Since the singular values are continuous functions of the elements in $G_u(u, \lambda)$, they are also continuous in λ. If

$$\sigma_{N-1} \geq \bar{\sigma} > 0$$

for all (u, λ) then the nullity of $G_u(u, \lambda)$ is at most one. If in addition $\sigma_N = 0$ then u_N spans the left nullspace of $G_u(u, \lambda)$. From the direct sum

$$Ker(G_u^T) \oplus Range(G_u) = R^N$$

we see that $G_\lambda(u_0, \lambda_0)$ is not in the $Range(G_u)$ if and only if $G_\lambda^T u_N \neq 0$. Hence we have a new, equivalent definition of simple fold.

Definition 3.1 (Simple Fold via SVD). *Let (u_0, λ_0) be a solution of $G(u, \lambda) = 0$, and let u_N be a left singular vector of $G_u(u_0, \lambda_0)$ associated with σ_N.*

Then (u_0, λ_0) is a **simple fold** *if*

- $dim(Ker(G_u(u_0, \lambda_0))) = 1$ *and*
- $u_N^T G_\lambda(u_0, \lambda_0) \neq 0$.

Continuity of $G_\lambda^T u_N$ implies that there is $\alpha > 0$ such that for all (u, λ)

$$\max\left(\sigma_N^2, |u_N^T G_\lambda|^2 \frac{\text{gap}}{\text{gap} + \xi^2}\right) \geq \alpha > 0,$$

where

$$\text{gap} \equiv \sigma_{N-1}^2 - \sigma_N^2, \qquad \text{and} \quad \xi \equiv |u_N^T G_\lambda| + \|(I - u_N u_N^T) G_\lambda\|.$$

THEOREM 3.2. *Let $\bar{\Omega}$ be the closure of an open subset $\Omega \in R^{N+1}$, and let G be continuously differentiable in $\bar{\Omega}$. Let $x_0 = (u_0, \lambda_0)$ in $\bar{\Omega}$ be a solution to $G(u_0, \lambda_0) = 0$, and $\mathcal{N}(x_0, s_0) = 0$ with $\|\dot{x}_0\| = 1$. Let $\tau \geq 0$ be such that $\|G_u \dot{u}_0 + G_\lambda \dot{\lambda}_0\| \leq \tau$.*

Assume that for all (u, λ) in $\bar{\Omega}$ there exists $\alpha > 0$ such that

$$\sigma_{N-1} > 0, \qquad \max\left\{\sigma_N^2,\, (u_N^T G_\lambda)^2 \, \frac{\text{gap}}{\text{gap} + \xi^2}\right\} \geq \alpha,$$

where

$$\text{gap} \equiv \sigma_{N-1}^2 - \sigma_N^2, \qquad \xi \equiv |u_N^T G_\lambda| + \|(I - u_N u_N^T) G_\lambda\|.$$

If $\tau < \alpha$, then for all $x = (u, \lambda)$ in $\bar{\Omega}$, the smallest singular value $\sigma_{\min}(F_x)$ of the Jacobian F_x of $F(x, s)$ is bounded from below with

$$\sigma_{\min}(F_x) \geq \sqrt{1 - \tau \max\left\{\frac{1}{\alpha}, 1\right\}}.$$

We postpone the proof of Theorem 3.2 until §3.1 in order to derive an auxiliary result first.

3.1. Lower Bound for the Smallest Eigenvalue. We derive a lower bound for the smallest eigenvalue of the rank-one update $A + yy^T$, where A is a real symmetric positive semi-definite matrix of order N, and y is a real $N \times 1$ vector.

Let $\beta_1 \geq \ldots \geq \beta_N$ be the eigenvalues of A. Weyl's monotonicity theorem [19, Theorem (10.3.1)] implies bounds for the smallest eigenvalue of $A + yy^T$:

$$\beta_N \leq \lambda_{\min}(A + yy^T) \leq \beta_{N-1}.$$

Intuitively one would expect that $\lambda_{\min}(A + yy^T)$ is larger if y is close to an eigenvector of β_N. We confirm this by deriving lower bounds for $\lambda_{\min}(A + yy^T)$ that incorporate the angle between y and the eigenspace of β_N.

THEOREM 3.3. *Let A be an $N \times N$ real symmetric positive semi-definite matrix, u_N an eigenvector of A associated with β_N, $\|u_N\| = 1$, and $y \neq 0$ a real $N \times 1$ vector. Set $y_N \equiv u_N^T y$. Then*

$$\lambda_{\min}(A + yy^T) \geq \max\left\{\beta_N,\, y_N^2 \, \frac{\text{gap}}{\text{gap} + \xi^2}\right\} \tag{3.1}$$

where $\text{gap} \equiv \beta_{N-1} - \beta_N$ *and* $\xi \equiv |y_N| + \sqrt{\|y\|^2 - |y_N|^2}$.

Proof. We first show that

$$\lambda_{\min}(A + yy^T) \geq \min\{\beta_N + y_N^2 \frac{\text{gap}}{\text{gap} + \xi^2},\ \beta_{N-1} \frac{y_N^2}{\xi^2}\} \tag{3.2}$$

is lower bound for $\lambda_{\min}(A + yy^T) = \min_{\|x\|=1} x^T(A + yy^T)x$.

Let

$$A = U \begin{pmatrix} \beta_1 & & \\ & \ddots & \\ & & \beta_N \end{pmatrix} U^T$$

be an eigendecomposition of A, and x be any real vector with $\|x\| = 1$. Partition

$$U^T x = \begin{pmatrix} \bar{x} \\ x_N \end{pmatrix}, \qquad U^T y = \begin{pmatrix} \bar{y} \\ y_N \end{pmatrix}$$

so that $\xi = |y_N| + \|\bar{y}\|$. Then

$$x^T(A + yy^T)x \geq \beta_{N-1}\|\bar{x}\|^2 + \beta_N x_N^2 + (y^T x)^2.$$

If $\|\bar{x}\| \geq |y_N|/\xi$ then

$$x^T(A + yy^T)x \geq (\beta_{N-1} y_N^2)/\xi^2,$$

which proves the second part of the bound in (3.2).

If $\|\bar{x}\| < |y_N|/\xi$ then $|y_N| - \|\bar{x}\|\xi > 0$, and it makes sense to use $|x_N| \geq 1 - \|\bar{x}\|$ in

$$|y^T x| = |y_N x_N + \bar{y}^T \bar{x}| \geq |y_N x_N| - \|\bar{x}\|\|\bar{y}\| \geq |y_N| - \|\bar{x}\|\xi.$$

Hence

$$x^T(A + yy^T)x \geq \beta_{N-1}\|\bar{x}\|^2 + \beta_N x_N^2 + (y^T x)^2 \geq \beta_N + y_N^2 + (\text{gap} + \xi^2)\|\bar{x}\|^2 - 2\xi\|\bar{x}\||y_N|.$$

This is a function of $\|\bar{x}\|$ which has a minimum at $\|\bar{x}\| = |y_N|\xi/(\text{gap} + \xi^2)$. Hence

$$x^T(A + yy^T)x \geq \beta_N + y_N^2 \frac{\text{gap}}{\text{gap} + \xi^2},$$

which proves the first part of the bound in (3.2).

With the help of (3.2) we now show the desired bound (3.1). Weyl's theorem [19, Theorem (10.3.1)] implies $\lambda_{\min}(A + yy^T) \geq \beta_N$, which proves the first part of the bound in (3.1). For the second part of the bound in (3.1), we use the fact that the eigenvalues of A are non-negative, hence $\beta_{N-1} \geq \text{gap}$ and

$$\frac{\beta_{N-1}}{\xi^2} \geq \frac{\text{gap}}{\text{gap} + \xi^2}.$$

Substituting this into (3.2) gives the second part of the bound in (3.1)

$$\begin{aligned} \min(A + yy^T) &\geq \min\{\beta_N + y_N^2 \frac{\text{gap}}{\text{gap} + \xi^2},\ y_N^2 \frac{\beta_{N-1}}{\xi^2}\} \\ &\geq \min\{\beta_N + y_N^2 \frac{\text{gap}}{\text{gap} + \xi^2},\ y_N^2 \frac{\text{gap}}{\text{gap} + \xi^2}\} = y_N^2 \frac{\text{gap}}{\text{gap} + \xi^2}. \end{aligned}$$

□

The quantity gap in Theorem 3.3 is the absolute gap between the smallest and next smallest eigenvalues. The theorem shows that $\lambda_{\min}(A + yy^T)$ is likely to be larger if y has a substantial contribution in the eigenspace of β_N. The bound in Theorem 3.3 is tight when y is a multiple of u_N. That is, if $|u_N^T y| = \|y\|$ then $\lambda_{\min}(A + yy^T) = \min\{\beta_N + \|y\|^2, \beta_{N-1}\}$.

Now we are in a position to complete the proof of Theorem 3.2.

3.2. Proof of Theorem 3.2. Define the residual $r \equiv G_u\dot{u}_0 + G_\lambda\dot{\lambda}_0$ and form

$$F_x F_x^T = \begin{pmatrix} G_u & G_\lambda \\ \dot{u}_0^T & \dot{\lambda}_0 \end{pmatrix} \begin{pmatrix} G_u^T & \dot{u}_0 \\ G_\lambda^T & \dot{\lambda}_0 \end{pmatrix} = \begin{pmatrix} G_u G_u^T + G_\lambda G_\lambda^T & r \\ r^T & 1 \end{pmatrix}.$$

The eigenvalues of $F_x F_x^T$ are the squares of the singular values of F_x. Applying Theorem 3.3 to $G_u G_u^T + G_\lambda G_\lambda^T$ with $A = G_u G_u^T$, $y = G_\lambda$, $\beta_N = \sigma_N^2$, $\beta_{N-1} = \sigma_{N-1}^2$ and gap $= \sigma_{N-1}^2 - \sigma_N^2$ shows $\lambda_{\min}(G_u G_u^T + G_\lambda G_\lambda^T) \geq \alpha$. Hence we can write

$$\begin{pmatrix} G_u G_u^T + G_\lambda G_\lambda^T & 0 \\ 0 & 1 \end{pmatrix}^{-1} F_x F_x^T = I + E,$$

where $\|E\| \leq \tau \max\left\{\frac{1}{\alpha}, 1\right\}$. If $\tau < \min\{\alpha, 1\}$ then $\|E\| < 1$, $I + E$ is nonsingular, and

$$\frac{1}{\|(F_x F_x^T)^{-1}\|} \geq 1 - \tau \max\left\{\frac{1}{\alpha}, 1\right\}.$$

4. Newton-GMRES and Eigenvalue Clustering. This section discusses the performance of the inner GMRES iteration in the context of continuation with a Newton-GMRES nonlinear solver. Theorem 3.2 gives conditions under which the Jacobian matrix F_x of the reformulated problem is uniformly nonsingular. This implies GMRES is a practical candidate for making the linear solve in Newton's method when implementing pseudo-arclength continuation. While the results in the previous section address conditioning, they do not directly translate into the performance of iterative methods [7, 11, 21], especially in the non-normal case. However, we can go further to see that the eigenvalue clustering properties of the matrix F_x do not stray far from those of G_u.

Suppose the eigenvalues of G_u are nicely clustered (in the sense of [3, 14]). Even in the singular case, this would mean that the zero eigenvalue of G_u is an "outlier". We seek to show that adding the row and column does not significantly increase the number of outliers, and that we can then use the estimates in [3, 14].

One approach is to use the paradigm of [13]. The idea is that

$$G_u = I + K(u) + E \tag{4.1}$$

where K_u is a low-rank operator, say of rank p, and E is small. We then want to write F_x in the same way, and then compare the number of outliers by comparing the ranks of the K-terms.

Assume that E is small enough so that the eigenvalues of $I - K$ are "outliers" in the sense of [3]. Since the degree of the minimal polynomial of $I - K$ is at most $p + 1$, we have a bound for the sequence of residuals $\{r_l\}$ of the GMRES iteration of the form

$$\|r_{\hat{p}+k}\| \leq C\|E\|^k\|r_0\| \tag{4.2}$$

where $\hat{p} \leq p+1$ GMRES iterations are needed to kill the contribution of the outlying eigenvalues.

Theorem 4.1 states that that the spectral properties of F_x are similar to those of G_u.

THEOREM 4.1. *Let the assumptions of Theorem 3.2 hold. Assume that* (4.1) *holds with* $rank(K(u)) = p$. *Then there is* $\mathcal{K}(u)$ *having rank at most* $p+2$ *such that*

$$\|F_x - I - \mathcal{K}(u)\| \leq \|E\|.$$

Proof. We write [13]

$$F_x = I_{(N+1)\times(N+1)} + \begin{pmatrix} K & G_\lambda \\ \dot{u}^T & \dot{\lambda} \end{pmatrix} + \begin{pmatrix} E & 0 \\ 0 & 0 \end{pmatrix}.$$

The range of

$$\mathcal{K} = \begin{pmatrix} K & G_\lambda \\ \dot{u}^T & \dot{\lambda} \end{pmatrix}$$

is

$$\begin{pmatrix} Range(K) \\ 0 \end{pmatrix} + \text{span}\left\{\begin{pmatrix} G_\lambda \\ 0 \end{pmatrix}\right\} + \text{span}\left\{\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\}$$

and hence the rank of $\mathcal{K}$ is at most $p+2$. □

So, while the eigenvalues may change, we have not increased the degree of the minimal polynomial of the main term (K vs $\mathcal{K}$) beyond $p+3$. Hence, the methods of [3] can be applied to obtain a bound like (4.2) with $\hat{p} \leq p+3$.

5. Example: Chandrasekhar H-Equation. We now present an example of a solution path containing a simple fold. The equation of interest is called the Chandrasekhar H-equation [4, 11, 17] from radiative transfer theory:

$$H(\mu) = 1 + \frac{c}{2}H(\mu)\int_0^1 H(\nu)\frac{d\nu\mu}{\mu+\nu}. \tag{5.1}$$

The goal is to compute the l^1 norm of the solution to Equation (5.1) for various natural parameter values c. That is, we compute

$$\|H\|_1 = \int_0^1 H(\nu, c)\, d\nu$$

as a function of c. Integrating (5.1) with respect to μ yields

$$\|H\|_1 = 1 + \frac{c}{2}\int_0^1\int_0^1 \frac{H(\mu)H(\mu)\mu\, d\mu\, d\nu}{\mu+\nu} = 1 + \frac{c}{4}\|H\|_1^2,$$

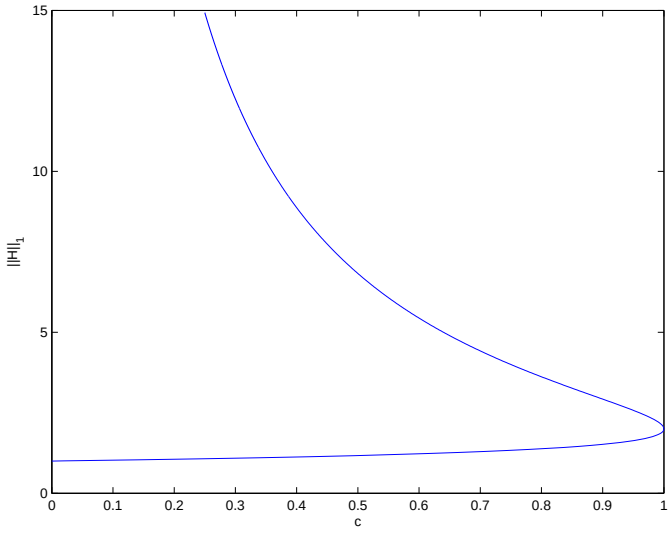
and so

$$\|H\|_1 = \frac{1 \pm \sqrt{1-c}}{c/2}. \tag{5.2}$$

Equation (5.2) tells us two interesting things. First, there can be no real solutions of the H-equation for $c > 1$, so there must be a singularity at $c = 1$, or else the implicit function theorem would tell us that we could continue past $c = 1$. Secondly, the $\pm$ gives us a hint that there may be two solutions, at least for $0 < c < 1$ (and there are!).

Figure 5.1 is a plot of $\|H\|_1$ against c. Notice how the curve bends around when $c = 1$, and how there are two solutions for each $0 < c < 1$. In fact, we are witnessing a simple fold at $c = 1$.

FIG. 5.1. $\|H\|_1$ *as a function of* c



5.1. Simple Fold at $c = 1$. For the H-equation, it is possible to compute the singularity analytically. Write the H-equation as

$$G(H, c)(\mu) = H(\mu) - \left(1 - \frac{c}{2}\int_0^1 \frac{\mu H(\nu)\, d\nu}{\mu + \nu}\right)^{-1}.$$

Taking the Fréchet derivative of F in the direction of w yields

$$G_H(H, c)w(\mu) = w(\mu) - \frac{\frac{c}{2}\int_0^1 \frac{\mu w(\nu)\, d\nu}{\mu + \nu}}{\left(1 - \frac{c}{2}\int_0^1 \frac{\mu H(\nu)\, d\nu}{\mu + \nu}\right)^2} = w(\mu) - \frac{c}{2}H(\mu)^2 \int_0^1 \frac{\mu w(\nu)\, d\nu}{\mu + \nu}.$$

Let $c = 1$, then (5.2) implies that

$$\int_0^1 H(\mu)\, d\mu = 2$$

and therefore

$$\begin{aligned}\tfrac{1}{2}\int_0^1 \frac{\nu H(\nu)\,d\nu}{\mu+\nu} &= \tfrac{1}{2}\int_0^1 H(\nu)\left(1-\frac{\mu}{\mu+\nu}\right)d\nu = 1-\int_0^1 \frac{\mu H(\nu)\,d\nu}{\mu+\nu}\\ &= H(\mu)^{-1}.\end{aligned}$$

Hence if $\phi(\mu)=\mu H(\mu)$,

$$G_H(H,1)\phi = 0,$$

and we have shown directly that G_H is singular at $c=1$.

One can apply Perron-Frobenius theory [8, 16] to show that the null space of G_H has dimension one, and hence is spanned by ϕ. The singularity at $c=1$ is a simple fold because

$$G_c(H,1)(\mu) = -H^2(\mu)\frac{1}{2}\frac{\mu H(\nu)\,d\nu}{\mu+\nu} = H^2(\mu)(H^{-1}(\mu)-1)$$

is not in the range of G_H. To see this note that

$$G_c(H,1)(\mu) = H^2(\mu)(H^{-1}(\mu)-1) \le 0$$

and vanishes only at $\mu=0$. The null space of G_H^T is the span of H^{-1}, which is strictly positive. Hence G_c is not orthogonal to the null space of G_H^T.

One can also show that G_H is nonsingular for all $c \neq 1$ by an argument even more tedious than the one above [10].

5.2. Smallest Singular Values. As a demonstration of the result in § 3, we calculate the smallest singular value of the Jacobian matrix associated with the augmented system for the H-equation with each continuation iteration. In the language of § 3, we find $\sigma_{\min}(F_{(H,c)})$ for various c where $F_{(H,c)}$ denotes the Jacobian of $\begin{pmatrix} G(H,c) \\ \mathcal{N}(H,c,s) \end{pmatrix}$. Figure 5.2 shows that the smallest singular value of $F_{(H,c)}$ for each c stays away from zero keeping $F_{(H,c)}$ nonsingular, even at the simple fold ($c=1$). The pseudo-arclength code used here uses a direct LU factorization of the Jacobian for the linear solve in Newton's method. The step in arclength is fixed at $ds=.5$, and we use a a secant predictor [9]. The integral is discretized with the composite midpoint rule and 200 nodes. The singular values are calculated using Matlab's `svd` command.

5.3. Computation with H-equation. The consequences of the remarks in § 4 are that for a problem like the H-equation, which is a nonlinear compact fixed point problem, the number of GMRES iterations per Newton step should be bounded. One must take this expectation with a grain of salt because as one moves along the path, the norm of the solution increases, and so the number of outliers may increase slowly. The observations we present illustrate this.

We use a Newton-GMRES version of pseudo-arclength continuation [5], fixing the step in arclength to $ds=.02$, using a secant predictor [9], and beginning the continuation at $c=0$, where the $H=1$ is the solution. The vector with coordinates all equal to one is

FIG. 5.2. $\sigma_{\min}(F_{(H,c)})$ *as a function of* c

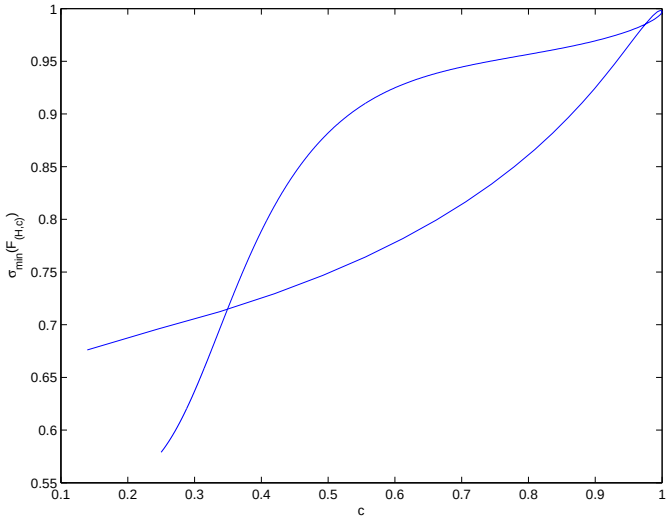
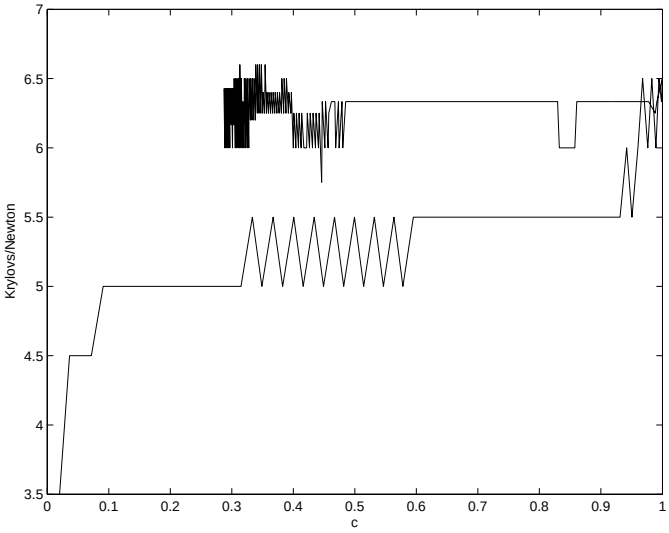


FIG. 5.3. *Krylov's per Newton*



the solution of the discrete problem as well. We discretize the integral with the composite midpoint rule using 400 nodes.

In Figure 5.3 we plot the average number of GMRES iterations per Newton iteration as a function of c. As one moves further on the path, the predictor becomes less effective, and the number of Newton iterations increase. Moreover, the norm of the solution also increases adding roughly one to the number of Krylov's per Newton.

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