Spectral Properties and Knot Removal for Interpolation by Pure Radial Sums

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Seminar für Angewandte Mathematik Eidgenössische Technische Hochschule CH-8092 Zürich Switzerland

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Abstract

We investigate some asymptotic spectral properties of the collocation matrix arising in interpolation by pure radial sums, and we provide some theoretical results that can be used for knot removal.

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§1. Introduction

Given an arbitrary finite subset $X = \{x_i\}_1^N$ of \mathbb{R}^d , where $d \geq 1$, of pairwise distinct points called "centres" and a set of real valued data $\Lambda = \{z_i\}_1^N$, the interpolation problem by radial basis functions consists of finding an interpolant of the form

$$\sigma(\cdot) = \sum_{i=1}^{N} \alpha_i \delta_{x_i} * \phi(\|\cdot\|^2) + p_k(\cdot) , \quad p_k \in \Pi_k(\mathbb{R}^d),$$
 (1)

such that $\sum_{i=1}^{N} \alpha_i \delta_{x_i} \perp \Pi_k(\mathbb{R}^d)$ and $\langle \sigma, \delta_{x_i} \rangle = z_i$, i = 1, 2, ..., N, where ϕ is a prescribed real-valued function in $C(\mathbb{R}_+)$, $\Pi_k(\mathbb{R}^d)$ is the space of d-variate polynomials of degree less than k, and $\|\cdot\|$ denotes the Euclidean norm on \mathbb{R}^d .

In matrix notation, solving the interpolation problem is equivalent to solving the linear system

$$\begin{pmatrix} A & U \\ U^T & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \Lambda^T \\ 0 \end{pmatrix}, \tag{2}$$

where

- $A = (\phi(||x_i x_j||^2))_{i,j=1}^N$ is the so-called collocation matrix and
- $U = (q_j(x_i))_{i=1,j=1}^{N-M}$ is the matrix associated with a given basis $\{q_j\}_{j=1}^{M}$

of
$$\Pi_k(\mathbb{R}^d)$$
 and $M = \dim \Pi_k(\mathbb{R}^d) = \binom{k-1+d}{d}$.

Obviously, a unique solution exists if

$$rank(U) = M \le N \tag{3}$$

$$\text{and} \qquad \varepsilon \alpha^T A \alpha > 0 \ , \ |\varepsilon| = 1, \quad \text{whenever} \quad U^T \alpha = 0 \ , \ \alpha \neq 0. \eqno(4)$$

Given a basis function ϕ and a fixed d, it is not always easy to see whether (4) is valid or not. In 1986, Micchelli [7] characterized certain smooth functions ϕ in terms of their derivatives for whom there exists M such that (4) holds for any d. The two main results of that paper are as follows. In order to state them, we begin with a definition.

Definition 1. A function $\phi \in C[0,\infty)$ is a conditionally strictly positive (negative) definite radial function of order k on \mathbb{R}^d if the condition (4) holds with $\varepsilon = +1$ ($\varepsilon = -1$) for any subset of centres X in \mathbb{R}^d .

We will denote the classes of such functions by $\mathcal{P}_k(\mathbb{R}^d)$ and $\mathcal{D}_k(\mathbb{R}^d)$, respectively, and, trivially, $\phi \in \mathcal{P}_k(\mathbb{R}^d)$ if and only if $-\phi \in \mathcal{D}_k(\mathbb{R}^d)$.

Theorem 1 [3,7]. The function ϕ is in $\mathcal{P}_k = \cap_{d\geq 1} \mathcal{P}_k(\mathbb{R}^d)$ if and only if $\phi \notin \Pi_{k+1}(\mathbb{R}_+)$ and ϕ is k-th order completely monotonic, i.e., $\phi \in C[0,\infty) \cap C^{\infty}(0,\infty)$ and $(-1)^j \phi^{(j)}(t) \geq 0$, t > 0, $j \geq k$.

Theorem 2 [7]. Suppose that $\phi(0) \geq 0$ and $\phi \in \mathcal{D}_1$ (we denote the set of all such functions by \mathcal{D}_1^+ by \mathcal{D}_1^+ from now on). Then, for any set of centres $X = \{x_i\}_1^N$, and any d,

$$(-1)^{N-1} \det \left(\phi(||x_i - x_j||^2) \right)_{i,j=1}^N > 0.$$

Moreover, we obtain from [9], denoting the *i*-th eigenvalue of the collocation matrix A, when the eigenvalues are ordered by size, by λ_i ,

$$\lambda_1 > 0 > \lambda_2 \ge \cdots \ge \lambda_N$$
.

It follows from the fact that the trace of the collocation matrix is the sums of its eigenvalues that

$$\lambda_1 = \max_{i=1,2,\dots,N} |\lambda_i| \ge \sum_{i=2}^N |\lambda_i|,$$

$$\lambda_2 = \min_{i=1,2,\dots,N} |\lambda_i|.$$

From now on we will focus on functions in the spaces \mathcal{P}_0 and \mathcal{D}_1^+ which allow interpolation by pure radial sums, *i.e.*, without a polynomial term added in (1), according to Theorems 1 and 2.

§2. Spectral behaviour when the number of centres increases

Let $X = \{x_i\}_1^N$ and $X' = \{x_i\}_1^{N'}$ be two sets of centres in \mathbb{R}^d for some d, where $N' > N \geq 2$, and let A, A' be the associated collocation matrices with respect to a function ϕ . We will denote by ρ_1 , ρ_2 (respectively ρ'_1 , ρ'_2) the maximal and minimal eigenvalues of A (respectively A') in modulus.

Lemma 1. A is irreducible whenever ϕ is in \mathcal{P}_0 or in \mathcal{D}_1^+ .

Proof: As a nonnegative matrix is irreducible if and only if its digraph is strongly connected, a sufficient condition for irreducibility is that the off-diagonal entries are all strictly positive. Clearly, $\phi \in \mathcal{D}_1^+$ implies that ϕ is strictly positive on $(0,\infty)$, thus A is irreducible. Now, if $\phi \in \mathcal{P}_0$ then ϕ does not have a zero on $(0,\infty)$ (in other words, ϕ is not compactly supported). Otherwise, the Laplace–Stieltjes representation of ϕ (see [11]),

$$\phi(t) = \int_0^\infty e^{-tu} d\alpha(u) , \quad t \ge 0,$$

where $d\alpha$ is a positive finite Borel measure on $[0, \infty)$, would lead to $\phi \equiv 0$, contradicting the fact that $\phi \in \mathcal{P}_0$.

Theorem 3. If ϕ is in \mathcal{P}_0 or in \mathcal{D}_1^+ then $\operatorname{cond}_2(A') > \operatorname{cond}_2(A)$, where $\operatorname{cond}_2(\cdot)$ denotes the spectral condition number (the condition number with respect to the Euclidean vector norm).

Proof: We show the result when $\phi \in \mathcal{D}_1^+$, the same arguments being valid in the other case. The matrix A is the leading principal submatrix of order N of A'. By Cauchy's interlacing property, $\rho'_1 \geq \rho_1 > 0 > \rho'_2 \geq \rho_2$, and, using Lemma 1 and the Frobenius theorem which states that the maximal eigenvalue of an irreducible matrix is (strictly) greater than the maximal eigenvalue of any of its principal submatrices, we obtain

$$\operatorname{cond}_2(A') = \frac{\rho_1'}{\rho_2'} > \frac{\rho_1}{\rho_2} = \operatorname{cond}_2(A). \quad \blacksquare$$

Theorem 4. The inequalities

$$0 < \rho_2 \le \phi(0) - \phi(q_N) < \max(\phi(0) + \phi(q_N), \phi(0) + (N-1)\phi(D_N))$$

$$\le \rho_1 \le \phi(0) + (N-1)\phi(q_N)$$

hold for $\phi \in \mathcal{P}_0$, and, for $\phi \in \mathcal{D}_1^+$,

$$0 < \rho_2 \le \phi(q_N) - \phi(0) \le \max(\phi(0) + \phi(D_N), \phi(0) + (N-1)\phi(q_N))$$

$$\le \rho_1 \le \phi(0) + (N-1)\phi(D_N),$$

where
$$D_N = \max_{1 \le i \ne j \le N} ||x_i - x_j||^2$$
, $q_N = \min_{1 \le i \ne j \le N} ||x_i - x_j||^2$.

Proof: We obtain the required bounds using that A is a nonnegative matrix which implies

$$\min_{1 \le i \le N} \sum_{j=1}^{N} \phi(\|x_i - x_j\|^2) \le \rho_1 \le \max_{1 \le i \le N} \sum_{j=1}^{N} \phi(\|x_i - x_j\|^2),$$

and with Cauchy's interlacing theorem applied to the two principal submatrices

$$\begin{pmatrix} \phi(0) & \phi(q_N) \\ \phi(q_N) & \phi(0) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \phi(0) & \phi(D_N) \\ \phi(D_N) & \phi(0) \end{pmatrix}. \quad \blacksquare$$

Corollary 1. If $\phi \in \mathcal{D}_1^+$, then $\operatorname{cond}_2(A)$ is not bounded from above as N increases.

Proof: It is a consequence of Theorem 4 that

$$\operatorname{cond}_2(A) = \frac{\rho_1}{\rho_2} \ge \frac{\phi(0) + (N-1)\phi(q_N)}{\phi(q_N) - \phi(0)} \ge \frac{(N-1)\phi(q_N)}{\phi(q_N)} = N - 1. \quad \blacksquare$$

Theorem 5. Assume $\phi \in \mathcal{P}_0$. Then $\operatorname{cond}_2(A)$ is bounded independently of the number of centres if and only if there exists q_0 such that $q_N \geq q_0 > 0$ and $\sum_{k=1}^{\infty} k^{d-1}\phi(k^2) < \infty$.

Proof: The necessity of the condition follows directly from Theorem 4 and the continuity of ϕ at the origin. For the converse, we use first a result of Narcowich and Ward [8] (see also [10]) which states that

$$\rho_2 \ge \Theta(q_N) = \int_0^\infty \vartheta(u) d\alpha(u) > 0,$$

where $\vartheta(u) = C_d(uq_N)^{-\frac{d}{2}} \exp(-\delta^2(uq_N)^{-1})$, C_d and δ being parameters depending only on d. So, if we add a centre x_0 to the set $\{x_i\}_1^N$ in such a way that

 $\min_{0 \le i \ne j \le N} ||x_i - x_j||^2 = q_0$, we would have $\rho_2 \ge \rho'_2 \ge \Theta(q_0) > 0$, where ρ'_2 denotes the minimal eigenvalue of $A' = (\phi(||x_i - x_j||^2))_{i,j=0}^N$. The rest of the proof which we omit consists of finding an upper bound for the spectral radius ρ_1 independently of N, using the assumption that ϕ decreases and an argument similar to the one in Jetter [4].

§3. On the eigenvalues of matrices depending on a parameter

Theorem 6. Let $X \subset \mathbb{R}^d$ be a fixed set of centres $\{x_i\}_1^N$. Let $(\phi_{\nu})_{\nu \in E}, E \subset \mathbb{R}$ be a family of functions in \mathcal{P}_0 or in \mathcal{D}_1^+ depending on a real parameter ν . We denote the collocation matrix associated with ϕ_{ν} by A_{ν} . If there exist ν_1 and ν_2 in E such that

$$\phi_{\nu_2}'(t) \neq \phi_{\nu_1}'(t) \quad \text{and} \quad (-1)^j [\phi_{\nu_2}{}^{(j)} - \phi_{\nu_1}{}^{(j)}](t) \ge 0 \quad , \quad t > 0, \ \ j \ge 0,$$

then the eigenvalues of the collocation matrices satisfy $\lambda_{i,A_{\nu_2}} > \lambda_{i,A_{\nu_1}}$, $i = 1,2,\ldots,N$, and $\operatorname{cond}_2(A_{\nu_2}) > \operatorname{cond}_2(A_{\nu_1})$ whenever $\phi_{\nu} \in \mathcal{D}_1^+$. Moreover, if $(\phi_{\nu})_{\nu}$ is (uniformly) continuous with respect to $\nu \in E$ for the (simple) uniform convergence topology, then $\lambda_{i,A_{\nu}}$ and $\operatorname{cond}_2(A_{\nu})$ are (uniformly) continuous with respect to ν .

Proof: The difference function $\Psi = \phi_{\nu_2} - \phi_{\nu_1}$, is nonconstant and 0-th order completely monotonic. Hence, as a consequence of Theorem 1, the collocation matrix $\delta A = \left(\Psi(||x_i - x_j||^2)\right)_{i,j=1}^N = A_{\nu_2} - A_{\nu_1}$ is strictly positive definite. Using Weyl's theorem on perturbations of eigenvalues of Hermitian matrices, we obtain that

$$\lambda_{i,A_{\nu_2}} \in [\lambda_{i,A_{\nu_1}} + \lambda_{N,\delta A}, \lambda_{i,A_{\nu_1}} + \lambda_{1,\delta A}], \quad i = 1, 2, \dots, N,$$

which implies that $\lambda_{i,A_{\nu_2}} > \lambda_{i,A_{\nu_1}}$, i = 1, 2, ..., N. In particular, for $\phi \in \mathcal{D}_1^+$,

$$\lambda_{1,A_{\nu_2}} > \lambda_{1,A_{\nu_1}} > 0 > \lambda_{2,A_{\nu_2}} > \lambda_{2,A_{\nu_1}};$$

hence $\operatorname{cond}_2(A_{\nu_2}) > \operatorname{cond}_2(A_{\nu_1})$. For the second assertion, we use the assumption that

$$\forall t > 0, \ \forall \nu_0 \in E, \ \forall \varepsilon > 0, \ \exists \eta > 0, \ \forall \nu \in E$$

$$|\nu_0 - \nu| < \eta \Longrightarrow |\phi_{\nu_0}(t) - \phi_{\nu}(t)| < \varepsilon.$$

Using successively the values $||x_i - x_j||^2$ for t, we obtain that $\forall \nu_0 \in E, \ \forall \varepsilon > 0, \ \exists \ \eta_{i,j} > 0$

$$|\nu_0 - \nu| < \eta_{i,j} \Longrightarrow |\phi_{\nu_0}(||x_i - x_j||^2) - \phi_{\nu}(||x_i - x_j||^2)| < \varepsilon.$$

With $\eta = \min_{i,j} \eta_{i,j}$, we have

$$|\nu_0 - \nu| < \eta \Longrightarrow \max_{i,j} |\phi_{\nu_0}(||x_i - x_j||^2) - \phi_{\nu}(||x_i - x_j||^2)| < \varepsilon.$$

This implies, for the Schur matrix norm $\|\cdot\|_S$, that

$$\|\delta A\|_{S} = \left\{ \sum_{i,j} [\phi_{\nu_0}(\|x_i - x_j\|^2) - \phi_{\nu}(\|x_i - x_j\|^2)]^2 \right\}^{1/2} < N\varepsilon.$$

Now, from Weyl's theorem,

$$\max_{i} |\lambda_{i,A_{\nu_0}} - \lambda_{i,A_{\nu}}| \le \lambda_{1,\delta A} = ||\delta A||_2 \le ||\delta A||_S.$$

Hence $\lambda_{i,A_{\nu}}$ and consequently $\operatorname{cond}_2(A_{\nu})$ depends continuously on ν . The uniform continuity is shown in the same manner.

Theorem 7. Let ϕ_{ν} be a function depending on a real parameter $\nu \in (a,b)$ and satisfying for any $\nu_2 > \nu_1$,

$$\phi'_{\nu_2}(t) \neq \phi'_{\nu_1}(t)$$
 and $(-1)^j [\phi_{\nu_2}{}^{(j)} - \phi_{\nu_1}{}^{(j)}](t) \ge 0$, $t > 0$, $j \ge 0$.

If $\phi_{\nu} \in \mathcal{P}_{0}$ and if there exists a function φ such that $\phi_{\nu}(t) \leq \varphi(t)$, t > 0, then $\operatorname{cond}_{2}(A_{\nu})$ is uniformly bounded as $\nu \to b$. Moreover, if $\phi_{\nu} \in \mathcal{D}_{1}^{+}$ and $\lim_{\nu \to b, t > 0} \phi_{\nu}(t) = \infty$, then $\lim_{\nu \to b} \operatorname{cond}_{2}(A_{\nu}) = \infty$.

Proof: For the first assertion, suppose that $\lim_{\nu \to b} \phi_{\nu}(0) = \phi_{b}(0) < \infty$. Then

$$||A_{\nu}||_{2} \le ||A_{\nu}||_{S} = \left\{ \sum_{i,j} [\phi_{\nu}(||x_{i} - x_{j}||^{2})]^{2} \right\}^{1/2} < N\phi_{b}(0), \quad \nu \in (a,b),$$

and, according to Theorem 6,

$$0 < ||A_{\nu}^{-1}||_2 \le ||A_{\nu_1}^{-1}||_2$$
, $\nu > \nu_1 > 0$.

Now if $\lim_{\nu \to b} \phi_{\nu}(0) = \infty$, then for any $\nu \in (a,b)$ we have $\max_{i} |\lambda_{i,\phi_{\nu}^{-1}(0)A_{\nu}} - 1| \le$

$$\left\{ \sum_{i \neq j} [\phi_{\nu}^{-1}(0)\phi_{\nu}(\|x_i - x_j\|^2)]^2 \right\}^{1/2} \le \left\{ \sum_{i \neq j} [\phi_{\nu}^{-1}(0)\varphi(\|x_i - x_j\|^2)]^2 \right\}^{1/2} \text{ and}$$

the last expression tends to 0 as $\nu \to b$ showing that

$$\operatorname{cond}_2(A_{\nu}) = \operatorname{cond}_2(\phi_{\nu}^{-1}(0)A_{\nu}) \to \operatorname{cond}_2(I) = 1$$

as $\nu \to b$ (I denotes the identity matrix of order N). For the second statement, we invoke Theorem 6 again, together with the inequality

$$||A_{\nu}||_{S} = \left\{ \sum_{i,j} [\phi_{\nu}(||x_{i} - x_{j}||^{2})]^{2} \right\}^{1/2} < N^{1/2} ||A_{\nu}||_{2}. \quad \blacksquare$$

Example: These results, when applied to the families of Hardy multiquadrics $(\phi_{\nu}(t))_{\nu>0} = ((t+\nu)^{1/2})_{\nu>0}$ and inverse multiquadrics $(\phi_{\nu}(t))_{\nu>0} = ((t+\nu)^{1/2})_{\nu>0}$, show that $\operatorname{cond}_2(A_{\nu})$ becomes unbounded with ν in the first case and tends to 1 in the second case. In the latter case, although it seems interesting that the condition number increases with ν , this is not a practically relevant case, since the matrix is going to be quasi-diagonal and the interpolating function is going to exhibit undesirable oscillations.

§4. Knot removal with radial basis functions

In this section, we study the effect of removing one centre at a time from a given interpolant or, equivalently, inserting one centre to a given interpolant. Due to a lack of space, we are not able to present the proofs of the results that follow. Instead, they will be published in [2].

Now, given points $\{x_j\}_1^N$ and $x_0 \notin \{x_j\}_1^N$, all in \mathbb{R}^d and pairwise distinct, we compare the uniform distance between the radial function interpolant σ' to $\{f(x_j)\}_1^N$ at $\{x_j\}_1^N$, and the interpolant σ^* that interpolates $f_{new} = f(x_0)$ at x_0 as well.

The result gives an upper bound on the uniform distance between σ' and σ^* that depends in a simple way on x_0 and f_{new} . Of course it depends on properties of the interpolation matrices $A' = \{\phi(\|x_j - x_k\|^2)\}_{j,k=1}^N$ and $A = \{\phi(\|x_j - x_k\|^2)\}_{j,k=0}^N$, and on the spacing h of the centres too. From now on, $\|\cdot\|_{\infty,\Omega}$ always denotes the uniform norm restricted to a compactum $\Omega \subset \mathbb{R}^d$ which contains all the centres including the new one.

In the following theorem, which provides an *a priori* error bound, we restrict ourselves to radial functions of the form

$$\phi(t) = (t+\nu)^{\beta/2}, \quad -d \le \beta < 0, \quad \nu > 0.$$
 (5)

Theorem 8. Under the stated conditions and for the radial function (5), we have the estimate

$$\|\sigma' - \sigma^*\|_{\infty,\Omega} \le C\rho_2^{-1/2} |f_{new} - \sigma'(x_0)| h^M,$$
 (6)

where $h = \max_{1 \leq j \leq N} \min_{1 \leq k \leq N} ||x_j - x_k||$, A is the collocation matrix including the centre x_0 standing for x_0 , ρ_2 is its smallest eigenvalue, M is arbitrary but integral and C is a positive constant independent of h, x_0 and f_{new} , but dependent on M.

This theorem gives a way to estimate the effect of inserting a knot x_0 to σ' which of course also allows to estimate the effect of removing a knot from σ^* .

More general results which give error estimates of the type (6) are available too. They apply to all polyharmonic splines where

$$\phi(t) = \begin{cases} t^{N-d/2} \log t, & d \text{ even, N} > \frac{d}{2}, \text{N an integer,} \\ t^{N-d/2}, & \text{otherwise with N} > \frac{d}{2}, \end{cases}$$
 (7)

and their shifted versions $\phi(t+\nu)$, of which (5) is a special case, but negative exponents are admitted in (5) because the shift avoids the singularity of (7) at the origin. Those results will be published elsewhere, as will computational experiments regarding the theoretical results. It should be noted that (7) and their shifted versions cover all of the most commonly studied and used radial functions.

This theoretical result allows us to decide when it is possible and when it is not possible to remove a given centre from the data set keeping a prescribed tolerance, for it is now sufficient to see whether the upper bound found in each of the cases is less than the prescribed tolerance. Unfortunately, this result is not constructive and, for practical purposes, we use the following technique which was tailor made for multiquadrics.

Theorem 9. We define discrete norms $\|\cdot\|_{d,p}$ and $\|\cdot\|_{d,\infty}$ on the set of radial functions spanned by multiquadrics, i.e., such that $\sigma = \sum_{i=1}^{N} \alpha_i \delta_{x_i} * \phi(\|\cdot\|^2)$ with $\|\sigma\|_{d,p} = \|\alpha\|_{d,p} = (\sum_{i=1}^{N} |\alpha_i|^p)^{1/p}$ and $\|\sigma\|_{d,\infty} = \|\alpha\|_{d,\infty} = \max |\alpha_i|$. Those norms are equivalent to the uniform norm $\|\cdot\|_{\infty}$.

Now, let σ be the multiquadric interpolating all the data and σ' the one interpolating all the data but in one point, say x_{i_0} .

Using some well known results on matrix norms and associated vector norms, we obtain the following upper bound for the relative error:

$$\frac{\|\sigma - \sigma'\|_{\infty,\Omega}}{\|\sigma\|_{\infty,\Omega}} \le C(\Omega)N\|A^{-1}\|_2 \frac{\|\sigma - \sigma'\|_{d,2}}{\|\sigma\|_{d,2}}$$

where A is the collocation matrix, N is the number of centres associated with σ , and $C(\Omega)$ is a geometric constant related to the diameter of Ω , specifically: $C(\Omega) = (\operatorname{diam}(\Omega)^2 + \nu)^{1/2}$, ν being the parameter in the basis function ϕ .

Let A' be the collocation matrix associated to σ' . A careful evaluation of the norm $||A'||_2$ leads to the upper bound

$$\|\sigma - \sigma'\|_{d,2} \le |\alpha_{i_0}| \{1 + \|A'\|_2 (N - 1)(\nu + D^2)\}^{1/2}$$

where $D = \max_{i,j} ||x_i - x_j||$. Now, using again the results of Narcowich and Ward, with $p = q^2(1 + (1 + q^2)^{1/2})^{-1}$ and q being the separation distance between the centres, we obtain an upper bound of the form

$$\frac{\|\sigma - \sigma'\|_{\infty,\Omega}}{\|\sigma\|_{\infty,\Omega}} \le K \frac{|\alpha_{i_0}|}{\|\alpha\|}.$$

Here, the constant K is

$$K = 5.95C(\Omega)Np^{-1}\exp(3p^{-1})\left\{1 + 5.95(N-1)(\nu+D^2)p^{-1}\exp(3p^{-1})\right\}^{1/2}.$$

This is more suitable for practical knot removal using multiquadrics, because it implies that for any i_0 such that

$$\frac{|\alpha_{i_0}|}{\|\alpha\|} \le \frac{\varepsilon}{K},$$

the relative error for σ is less than a given tolerance ε . Now, the usual techniques [5,6] for knot removal can be invoked.

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