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Sensitivity of the Lanczos recurrence to Gaussian quadrature data: How malignant can small weights be?

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ABSTRACT

Stability of passing from Gaussian quadrature data to the Lanczos recurrence coefficients is considered. Special attention is paid to estimates explicitly expressed in terms of quadrature data and not having weights in denominators. It has been shown that the recent approach, exploiting integral representation of Hankel determinants, implies quantitative improvement of D. Laurie's constructive estimate.

It has also been demonstrated that a particular implementation on the Hankel determinant approach gives an estimate being unimprovable up to a coefficient; the corresponding example involves quadrature data with a small but not too small weight. It follows that polynomial increase of a general case upper bound in terms of the dimension is unavoidable.

1. Introduction

Let

$$\mu(x) = \sum_{i=1}^{n} \omega_i \delta(x - \lambda_i), \quad \omega_1, \dots, \omega_n > 0, \lambda_1 < \lambda_2 < \dots < \lambda_n, \tag{1}$$

be a nonnegative measure with a finite support on the real line, having moments

$$s_j = \int x^j \mathrm{d}\mu(x), \quad j \in \mathbf{N}.$$

It induces the quadrature formula [1]

$$f \mapsto \sum_{i=1}^{n} \omega_i f(\lambda_i).$$

Introduce the polynomials Q_j, $\deg Q_j = j$, $0 \le j \le n-1$, orthonormal with respect to the measure μ and having positive leading coefficients. They obey the Lanczos recurrence [2]

$$\begin{aligned} &xQ_k(x) = \beta_{k+1} Q_{k+1}(x) + \alpha_{k+1} Q_k(x) + \beta_k Q_{k-1}(x) \quad (0 \le k \le n-2), \\ &\beta_k > 0, \qquad Q_{-1} \equiv 0, \qquad Q_0 = 1/\sqrt{s_0} \end{aligned} \tag{2}$$

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(Q_k can be considered as the Lanczos vectors of the Lanczos process in $L_{2,\mu}$ with the initial vector 1 (a constant function) and the operator of multiplication by x).

The mapping

$$(\lambda_1, \dots, \lambda_n; \omega_1, \dots, \omega_n) \mapsto (\alpha_1, \dots, \alpha_n; \beta_1, \dots, \beta_{n-1}) \tag{3}$$

is a popular object of investigation in the computational theory of orthogonal polynomials (see, e.g., [3]). Its stability was conjectured in [4].

A close problem, stated in [5] and called the Jacobi inverse eigenvalue problem (JIEP), is to determine α_i and β_j via λ_k and the $n-1$ eigenvalues of the principal lower $(n-1)\times(n-1)$ submatrix of the Jacobi matrix

$$J = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n-2} & \alpha_{n-2} & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{pmatrix}, \quad \alpha_k, \beta_k \in \mathbf{R}, \beta_k > 0. \tag{4}$$

JIEP is discussed in [6,7].

A qualitative perturbation bound for JIEP was established in [8] and probably the first constructive (though rather rough) one — in [9].

Realistic (at least, for not small weights) estimates appeared in [10,11]. These estimates contained either weights in denominators or derivatives of orthonormal or Lagrange interpolation polynomials. Note that such an estimate was an auxiliary tool in [10], it enabled the authors of that work to determine how to choose modified moments (see [3]).

It seems that the first realistic perturbation bound in terms of quadrature data and without weights in denominators was obtained in [12] and was also a secondary product there. Actually, D. Laurie modified the Gragg–Harrod algorithm [13] for (3), additionally using algorithms from works [14–16]. The resulting algorithm takes ω_i $(1 \le i \le n)$, $\lambda_{j+1}-\lambda_j$ $(1 \le j \le n-1)$ and produces $\alpha_i - \lambda_1$, β_j by means of additions, multiplications and divisions of positive numbers.

Let the symbol $\mathtt{RP}$ denote relative perturbation: $\mathtt{RP}\, a = |\widetilde{a}/a - 1|$, where $\widetilde{a}$ is a perturbed value of a quantity $a \neq 0$. Analogously, let the symbol $\mathtt{AP}$ denote absolute perturbation: $\mathtt{AP}\, a = |\widetilde{a} - a|$.

Theorem 1 (*Laurie [12]*). *If $\varepsilon > 0$ and*

$$\mathtt{RP}\, \omega_i \le \varepsilon, \quad 1 \le i \le n, \qquad \mathtt{RP}\, (\lambda_{j+1} - \lambda_j) \le \varepsilon, \quad 1 \le j \le n-1, \tag{5}$$

then

$$\mathtt{RP}\, \beta_j^2 \le \frac{9}{2} n^2 \varepsilon + O(n\varepsilon), \quad 1 \le j \le n-1, \tag{6}$$

$$\mathtt{RP}\, (\alpha_i - \lambda_1) \le \frac{9}{2} n^2 \varepsilon + O(n\varepsilon), \quad 1 \le i \le n. \tag{7}$$

In [17] we proposed a very simple approach based on the use of Hankel determinants

$$H_k = \begin{vmatrix} s_0 & s_1 & \dots & s_{k-1} \\ s_1 & s_2 & \dots & s_k \\ \vdots & \vdots & \dots & \vdots \\ s_{k-1} & s_k & \dots & s_{2k-2} \end{vmatrix} \quad \text{and} \quad G_k = \begin{vmatrix} s_1 & s_2 & \dots & s_k \\ s_2 & s_3 & \dots & s_{k+1} \\ \vdots & \vdots & \dots & \vdots \\ s_k & s_{k+1} & \dots & s_{2k-1} \end{vmatrix}.$$

They possess integral[1] representations [18]

$$H_k = \sum_{t_1 < \dots < t_k, t_1, \dots, t_k \in \{\lambda_1, \dots, \lambda_n\}} \prod_{1 \le i < j \le k} (t_j - t_i)^2 \prod_{i=1}^{k} \mu(t_i) \tag{8}$$

and

$$G_k = \sum_{t_1 < \dots < t_k, t_1, \dots, t_k \in \{\lambda_1, \dots, \lambda_n\}} \prod_{1 \le i < j \le k} (t_j - t_i)^2 \prod_{i=1}^{k} (t_i \mu(t_i)). \tag{9}$$

[1] Our situation is discrete, so integrals turn into finite sums.

One also has expressions [19]

$$\beta_j^2 = \frac{H_{j-1}H_{j+1}}{H_j^2}, \quad 1 \le j \le n-1, \tag{10}$$

$$\alpha_j = \frac{H_j G_{j-2}}{H_{j-1}G_{j-1}} + \frac{H_{j-1}G_j}{H_j G_{j-1}}, \quad 1 \le j \le n. \tag{11}$$

By the way, these expressions were exploited by H. Rutishauser in the formulation of QD-algorithm [20]. Formulae (8)–(11) enable one to easily bound the perturbation of the Lanczos recurrence under various assumptions on quadrature data's perturbation, so this approach is flexible. These formulae imply once again that small weights $\omega_i \ll 1$ do not cause a catastrophe provided $\mathrm{RP}\,\omega_i \ll 1$.

Note that the Hankel determinant approach is suitable also for the unitary Hessenberg inverse eigenvalue problem (see [17]), whose description and underlying algorithms can be found in [21,7,22].

Stability estimates for (3), intended for handling the discrete inverse Sturm–Liouville problem, can be found in [23,24]. The estimates contain weights in denominators, which is all right for Sturm–Liouville.

In Section 2 we shall take Laurie's conditions (5) and a little strengthen bounds (6)–(7).

In Section 3 we shall show that moderately small weights can influence the sensitivity to eigenvalue perturbations, which implies the linear increase of some sensitivity bound in terms of the dimension n.

2. Strengthening D. Laurie's estimates

To shorten further formulae, we introduce the family of functions (it will enable us to avoid taking care of $O(\delta^2)$ terms; cf. [25])

$$\overset{m}{\mathcal{D}}(\delta) = \frac{\delta}{1-m\delta}, \quad 0 \le \delta < \frac{1}{m}, \quad m \ge 1, \qquad \mathcal{D} = \overset{1}{\mathcal{D}}. \tag{12}$$

These monotonically increasing functions possess the following simple properties:

$$\overset{m}{\mathcal{D}}(\delta) = \delta + O(\delta^2) \quad \text{as } \delta \to +0;$$

$$\mathcal{D}\left[\overset{m}{\mathcal{D}}(\delta)\right] = \overset{m+1}{\mathcal{D}}(\delta), \quad 0 \le \delta < \frac{1}{m+1}; \tag{13}$$

$$\overset{m}{\mathcal{D}}(\delta) \le \overset{m+1}{\mathcal{D}}(\delta), \quad 0 \le \delta < \frac{1}{m+1}; \tag{14}$$

$$\overset{m}{\mathcal{D}}(\delta_1) + \overset{m}{\mathcal{D}}(\delta_2) \le \overset{m}{\mathcal{D}}(\delta_1+\delta_2), \quad \delta_1 \ge 0, \delta_2 \ge 0, \delta_1+\delta_2 \le \frac{1}{m}; \tag{15}$$

$$\mathrm{RP}\prod_{i=1}^k a_i \le \mathcal{D}\left(\sum_{i=1}^k \mathrm{RP}\,a_i\right); \tag{16}$$

$$\text{if } \mathrm{RP}\,a \le \mathcal{D}(\delta), \quad \text{then } \mathrm{RP}\,\frac{1}{a} \le \overset{2}{\mathcal{D}}(\delta). \tag{17}$$

Remark 1. Estimates with $\overset{m}{\mathcal{D}}$ are valid when the quantities under the $\overset{m}{\mathcal{D}}$ symbols obey the inequality in (12).

Theorem 2. *Let $\varepsilon > 0$ and conditions (5) hold. Then*

$$\mathrm{RP}\,\beta_k^2 \le \overset{3}{\mathcal{D}}[(4k^2+2)\varepsilon], \quad 1 \le k \le n-1. \tag{18}$$

If additionally $\lambda_1 = \widetilde{\lambda}_1 = 0$, then

$$\mathrm{RP}\,\alpha_k \le \overset{3}{\mathcal{D}}[(4k^2-2k+3)\varepsilon], \quad 1 \le k \le n. \tag{19}$$

Proof. Since an individual addend in (8) includes k^2 factors with $\mathrm{RP} \le \varepsilon$ each, we have

$$\mathrm{RP}\,H_k \le \mathcal{D}(k^2\varepsilon) \tag{20}$$

in view of (16), due to the simple facts that

$$\mathrm{RP}\,(a+b) \le \max\{\mathrm{RP}\,a, \mathrm{RP}\,b\}, \quad a, b > 0,$$

and that each addend occurring in (8) is positive. Then representation (10), combined with (13)–(17), implies

$$\operatorname{RP} \beta_k^2 \le \mathcal{D}\left(\operatorname{RP} H_{k-1} + \operatorname{RP} H_{k+1} + 2\operatorname{RP} H_k^{-1}\right)$$
$$\le \mathcal{D}\left\{\mathcal{D}[(k-1)^2\varepsilon] + \mathcal{D}[(k+1)^2\varepsilon] + 2 \overset{2}{\mathcal{D}} (k^2\varepsilon)\right\} \le \overset{3}{\mathcal{D}} [(4k^2+2)\varepsilon].$$

Inequality (18) has been established.

If $\lambda_1 = \underset{\smile}{\lambda}_1 = 0$, then, by induction, $\operatorname{RP} \lambda_i \le \varepsilon$, $i \ge 2$. In representation (9) the addends with a factor of $\lambda_1 = 0$ vanish; the other addends consist of $k(k+1)$ factors with $\operatorname{RP} \le \varepsilon$ each. Thus,

$$\operatorname{RP} G_k \le \mathcal{D}[k(k+1)\varepsilon].$$

In conjunction with (20) this gives

$$\operatorname{RP} \frac{H_k G_{k-2}}{H_{k-1} G_{k-1}} \le \overset{3}{\mathcal{D}} \left\{[k^2 + (k-2)(k-1) + (k-1)^2 + (k-1)k]\varepsilon\right\}$$
$$= \overset{3}{\mathcal{D}} [(4k^2 - 6k + 3)\varepsilon]. \tag{21}$$

Analogously,

$$\operatorname{RP} \frac{H_{k-1} G_k}{H_k G_{k-1}} \le \overset{3}{\mathcal{D}} \left\{[(k-1)^2 + k(k+1) + k^2 + (k-1)k]\varepsilon\right\}$$
$$= \overset{3}{\mathcal{D}} [(4k^2 - 2k + 1)\varepsilon]. \tag{22}$$

Accounting (11) and comparing (21) with (22), obtain (19). □

3. Influence of a moderately small weight on the sensitivity to perturbation of the corresponding eigenvalue

Introduce the eigenvalue separation

$$d_i = \min\{|\lambda_i - \lambda_j| \mid 1 \le j \le n, j \ne i\}.$$

Theorem 3. *Let $\operatorname{AP} \lambda_j \le \varepsilon$ for a fixed j, $1 \le j \le n$, while all the remaining eigenvalues and all the weights are frozen. Then the estimate*

$$\operatorname{RP} \beta_k^2 \le \overset{3}{\mathcal{D}} \left[\frac{\max\{8k-8, 2\}\varepsilon}{d_j}\right] \tag{23}$$

holds.

Proof. Any addend in (8) contains $\le 2(k-1)$ perturbed factors, with $\operatorname{RP} \le \varepsilon/d_j$ each, so

$$\operatorname{RP} H_k \le \mathcal{D}\left[\frac{2(k-1)\varepsilon}{d_j}\right].$$

This in conjunction with (10) implies (23). □

The next theorem shows that the k-dependent multiple may not be omitted in (23). Again, we assume that only λ_n is perturbed in the spectrum.

Theorem 4. *There exists a sequence of discrete measures μ_n of type (1) and of size $n = 4, 5, \ldots$, such that for any n $d_n \ge 1$ and*

$$\frac{1}{\beta_{n-2}^2}\left|\frac{\mathrm{d}\beta_{n-2}^2}{\mathrm{d}\lambda_n}\right| \ge cn, \tag{24}$$

where $c > 0$ is an absolute constant.

Proof. We shall modify [11, example 4]. First, we take the quadrature

$$\lambda_{n-k} = \cos\left[\frac{2k-1}{2(n-1)}\pi\right], \qquad \omega_k = \frac{1}{n-1}, \quad k = 1, \ldots, n-1,$$

with $n-1$ nodes and weights. The corresponding orthonormal polynomials equal

$$\pi_k = \begin{cases} T_0 & \text{if } k = 0, \\ \sqrt{2}\, T_k & \text{if } 1 \le k \le n-2, \end{cases} \tag{25}$$

with T_k the first kind Chebyshev polynomials. Note that the last off-diagonal component of the corresponding Jacobi matrix is $\beta_{n-2}^{(0)} = 1/2$.

Now we add a node $\lambda_n = \tau > 1$ supplied with a weight $y > 0$. We shall study the sensitivity of β_{n-2} to the perturbation of τ around the value 2. The key point is to properly choose the weight y.

Lemma 7.15 from [26] gives the representation

$$\left(\frac{\beta_{n-2}}{\beta_{n-2}^{(0)}}\right)^2 = \frac{\left[1 + y\sum_{i=0}^{n-4}\pi_i(\tau)^2\right]\left[1 + y\sum_{i=0}^{n-2}\pi_i(\tau)^2\right]}{\left[1 + y\sum_{i=0}^{n-3}\pi_i(\tau)^2\right]^2},$$

which, in terms of $\rho = \Phi(\tau)^2$ ($\Phi(\tau) = \tau + \sqrt{\tau^2 - 1}$ is the inverse Zhukovsky function), can be rewritten as

$$\left(\frac{\beta_{n-2}}{\beta_{n-2}^{(0)}}\right)^2 = \frac{R_{n-4}(\rho)R_{n-2}(\rho)}{R_{n-3}(\rho)^2},$$

where

$$R_j(\rho) = 1 + yS_j(\rho), \qquad S_j(\rho) = \sum_{i=0}^{j}\pi_i(\tau)^2. \tag{26}$$

Elementary calculations, considering (26), (25) and the representation

$$T_k(\tau) = \frac{\Phi(\tau)^k + \Phi(\tau)^{-k}}{2}, \quad k \in \mathbf{N}$$

(see [2, Appendix B]), give us

$$\begin{aligned} S_j(\rho) &= 2\sum_{i=0}^{j}\frac{\rho^i + \rho^{-i} + 2}{4} - 1 \\ &= \sum_{i=0}^{j}\frac{\rho^i + \rho^{-i}}{2} + j = \frac{1}{2}\sum_{i=-j}^{j}\rho^i + j + \frac{1}{2} \\ &= \frac{1}{2}\rho^{-j}\frac{\rho^{2j+1} - 1}{\rho - 1} + j + \frac{1}{2} = \frac{\rho^{j+1} - \rho^{-j}}{2(\rho - 1)} + j + \frac{1}{2} \end{aligned} \tag{27}$$

and, further,

$$\begin{aligned} S_j'(\rho) &= \frac{1}{2}\left(\frac{\rho^{j+1} - \rho^{-j}}{\rho - 1}\right)' \\ &= \frac{(\rho^{j+1} - \rho^{-j})'(\rho - 1) - (\rho^{j+1} - \rho^{-j})}{2(\rho - 1)^2} \\ &= \frac{[(j+1)\rho^j + j\rho^{-j-1}](\rho - 1) - \rho^{j+1} + \rho^{-j}}{2(\rho - 1)^2} \\ &= \frac{(j+1)\rho^{j+1} + j\rho^{-j} - (j+1)\rho^j - j\rho^{-j-1} - \rho^{j+1} + \rho^{-j}}{2(\rho - 1)^2} \\ &= \frac{j\rho^{j+1} + (j+1)\rho^{-j} - (j+1)\rho^j - j\rho^{-j-1}}{2(\rho - 1)^2}. \end{aligned} \tag{28}$$

Put

$$\zeta = \Phi(2)^2 \quad \text{and} \quad y = a\zeta^{-n},$$

where $a > 0$ is a constant. By virtue of (26)–(28), we have as $n \to +\infty$ and $j = n + O(1)$:

$$\begin{aligned} R_j(\zeta) &= 1 + yS_j(\zeta) = 1 + a\zeta^{-n}\left[\frac{\zeta^{j+1} - \zeta^{-j}}{2(\zeta - 1)} + j + \frac{1}{2}\right] \\ &= 1 + \frac{a\zeta^{j+1-n}}{2(\zeta - 1)} + O(n\zeta^{-n}) \end{aligned} \tag{29}$$

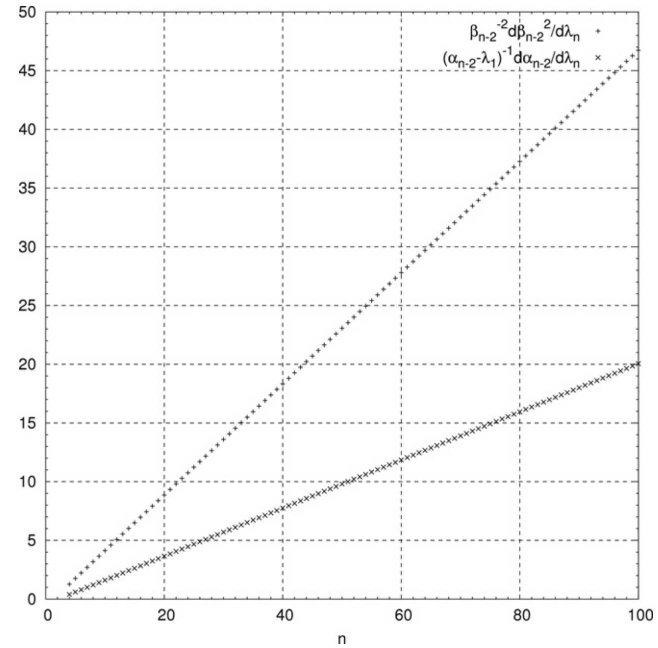

Fig. 1. Sensitivity of β_{n-2} and α_{n-2} to the perturbation of λ_n; $\zeta = \Phi(2)^2$, $a = 1090$.

and

$$\begin{aligned} R_j'(\zeta) &= yS_j'(\zeta) = \frac{a}{2}\zeta^{-n}\frac{j\zeta^{j+1} - (j+1)\zeta^j}{(\zeta-1)^2} + O(n\zeta^{-n}) \\ &= \frac{a}{2}\left[\frac{j\zeta^{j-n}}{\zeta-1} - \frac{\zeta^{j-n}}{(\zeta-1)^2}\right] + O(n\zeta^{-n}) = \frac{a}{2}\frac{n\zeta^{j-n}}{\zeta-1}\left[1 + O\left(\frac{1}{n}\right)\right]. \end{aligned} \tag{30}$$

Since

$$\left(\frac{R_{n-4}R_{n-2}}{R_{n-3}^2}\right)' = \frac{R_{n-4}'R_{n-2} + R_{n-4}R_{n-2}'}{R_{n-3}^2} - 2\frac{R_{n-4}R_{n-3}'R_{n-2}}{R_{n-3}^3},$$

then it follows from (29) and (30) that

$$\begin{aligned} \left(\frac{R_{n-4}R_{n-2}}{R_{n-3}^2}\right)'(\zeta) &= \frac{\frac{a}{2}\frac{n\zeta^{-4}}{\zeta-1}\left[1 + \frac{a\zeta^{-1}}{2(\zeta-1)}\right]}{\left[1 + \frac{a\zeta^{-2}}{2(\zeta-1)}\right]^2}\left[1 + O\left(\frac{1}{n}\right)\right] + \frac{\left[1 + \frac{a\zeta^{-3}}{2(\zeta-1)}\right]\frac{a}{2}\frac{n\zeta^{-2}}{\zeta-1}}{\left[1 + \frac{a\zeta^{-2}}{2(\zeta-1)}\right]^2}\left[1 + O\left(\frac{1}{n}\right)\right] \\ &\quad - 2\frac{\left[1 + \frac{a\zeta^{-3}}{2(\zeta-1)}\right]\left[1 + \frac{a\zeta^{-1}}{2(\zeta-1)}\right]\frac{a}{2}\frac{n\zeta^{-3}}{\zeta-1}}{\left[1 + \frac{a\zeta^{-2}}{2(\zeta-1)}\right]^3}\left[1 + O\left(\frac{1}{n}\right)\right] \\ &= b(a,\zeta)n + O(1). \end{aligned}$$

It is easy to check numerically that, say, the coefficient $b(a,\zeta) \approx 0.473 \neq 0$ when $a = 1090$.

To obtain (24), it remains to note that $\Phi(\tau) > 0$ and $\Phi'(\tau) > 0$ when $\tau > 1$, so turning back to the spectral variable τ does not spoil the sensitivity analysis, and to note that $\beta_{n-2} \leq 2$ in the given example. $\square$

For numerical illustration to Theorem 4 see line + in Fig. 1.

Remark 2. The same technique would enable one to investigate the sensitivity of recurrence coefficients α_j from (2) (diagonal components of matrix (4)) to the perturbation of λ_n. The mentioned lemma by P. Nevai gives (account $\alpha_{n-2}^{(0)} = 0$)

$$\alpha_{n-2} = y\frac{\beta_{n-2}\pi_{n-3}(\tau)\pi_{n-2}(\tau)}{1 + y\sum_{i=0}^{n-3}\pi_i(\tau)^2} - y\frac{\beta_{n-3}\pi_{n-4}(\tau)\pi_{n-3}(\tau)}{1 + y\sum_{i=0}^{n-4}\pi_i(\tau)^2},$$

which can be used to this end. Please refer to line $\times$ in Fig. 1 for the result of the calculation.

4. Conclusive remarks

In [17] a very simple approach for obtaining stability bounds was proposed. It was based on the integral representation of Hankel determinants. In the first half of this paper we have used this approach to improve the stability bound from [12]. The upper bounds under consideration have exhibited polynomial growth in terms of a dimension n.

In the second half we have shown that, in the general case, polynomial increase of bounds is unavoidable: a small weight may increase the sensitivity to perturbation of the corresponding eigenvalue. In this sense, small (even unperturbed) weights do complicate the life (though this complication is rather moderate). If estimates uniform in n are required in any application, then specific features of the spectrum must be exploited (as, e. g., in [24]).

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