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A Statistical Analysis of the Numerical Condition of Multiple Roots of Polynomials

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Abstract—Componentwise and normwise condition numbers of an m-tuple root x_0 of a polynomial $p(x)$ that are appropriate for measurement and experimental inaccuracies are derived. These new condition numbers must be compared with the established condition numbers, which are appropriate for quantifying the effect of roundoff errors due to floating point arithmetic. It is shown that the condition numbers that are derived in this paper may be considered average case (as opposed to worst case) because extensive use is made of the expected values of random variables and functions of random variables. Specifically, it is assumed that each coefficient of $p(x)$ is perturbed by an independent zero mean Gaussian random variable, and a measure of the condition of x_0 is defined as the ratio of the expected value of its relative error to the expected value of the relative error in the coefficients of $p(x)$, defined in both the componentwise and normwise forms. It is shown that this distinction between the componentwise and normwise condition estimates is important because they may differ by several orders of magnitude, depending on the coefficients of the polynomial. The cause of ill-conditioning of multiple roots is considered and it is shown that the situations $m = 1$ and $m > 1$ must be treated separately. Computational experiments that illustrate the theoretical results are presented.

Keywords—Polynomial roots, Average case componentwise condition number, Average case normwise number.

1. INTRODUCTION

Many problems in applied mathematics and engineering require the determination of the roots of a polynomial. Typically, these problems occur in geometric modelling, computer graphics, robotics, and signal processing.

- Important operations in geometric modelling and computer graphics include the computation of the points of intersection of parametric curves, the processing of the curve of intersection of parametric surface patches, and ray tracing parametric surfaces [1], all of which can be reduced to the determination of the real roots of a univariate polynomial.
- The inverse kinematics problem in robotics requires the solution of a system of multivariate polynomial equations whose coefficients represent (either explicitly or implicitly) the lengths and angles of the segments of the robot and the relative positions of the objects to be manipulated [2].
- Many problems in signal processing, including spectral factorisation (for filter and wavelet design, and spectral estimation), phase unwrapping, and the construction of a cascade of lower-order systems, require the accurate and rapid solution of polynomial equations [3].

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Furthermore, multiple roots of polynomials appear in several applications.

- Blends are an important requirement in the design of mechanical components because they allow one surface to merge smoothly into another surface, thereby eliminating sharp corners and stress concentration centres, which can cause mechanical failure. Blends are also required for reasons of aesthetic appeal, and they are characterised by tangency conditions, and therefore multiple roots, between the touching surfaces.
- The accuracy of the approximation of a function $f(t)$ by a scaling function and a wavelet basis is governed by ζ, the number of zeros of a lowpass filter $H(\omega)$ at $\omega = \pi$ [4, Chapter 7]. The larger the value of ζ, the smoother the scaling function and the more stable the lowpass filter under iteration.

If the data in these applications are derived from experimental measurements, they are subject to uncertainty and must, therefore, be regarded as typical values; another set of coefficients that lies within their domain of uncertainty is equally valid. This leads naturally to the concept of numerical condition, which is a measure of the sensitivity of the solution to perturbations in the input data. An estimate of the numerical condition of a computed quantity is a necessary requirement because it quantifies its computational reliability; a computed quantity whose condition number is high implies that it is very sensitive to minor perturbations in the data, but a low condition number is indicative of a solution that is only weakly dependent on these minor perturbations.

The difficulties that arise in computing high-order roots of polynomials are considered in [5], and it is shown that clustering may be used to obtain a numerically stable approximation to a high-order root. A cluster of roots is defined as a tightly localised and isolated set of approximate roots which are assumed to be the computed values of a multiple root. For example, the computed roots of the polynomial $(x-\alpha)^m$ lie in a localised cluster that is centred approximately at $x = \alpha$. Since the arithmetic mean of a cluster of roots is much less sensitive to small perturbations in the coefficients of the polynomial than are the individual roots in the cluster, the mean of the cluster may be a much better approximation to the true value of the multiple root than are any members of the cluster. This procedure depends on the identification of the correct cluster, but this is in general a difficult task [6]. This difficulty is demonstrated in [5] by the polynomial $(x - 0.5)(x^{10} - \eta)$. If $\eta = 2^{-10}$, there is a double root $x_{1,2} = 0.5$, a simple root $x_3 = -0.5$, and the remaining eight roots form four complex conjugate pairs. The two roots at 0.5 belong to two different clusters, but it is not obvious from plotting these roots in the complex plane that this is the correct choice.

The measurement and experimental errors discussed above are one source of uncertainty that must be considered when determining the computational reliability of a numerical result. Another source, the effect of roundoff errors due to floating point arithmetic, must be considered and it is shown in Section 2 that it is insignificant compared to measurement and experimental errors in most practical applications. Componentwise and normwise expressions for the numerical condition of a root of a polynomial, using an error model that is appropriate for measurement and experimental inaccuracies, are derived in Section 3, and the cause of ill-conditioning of multiple roots is considered in Section 4. The distinction between the componentwise and normwise measures is considered in Section 5, and it is shown that they may differ by several orders of magnitude, depending upon the coefficients of the polynomial. Examples that illustrate the theoretical results are presented in Section 6, and Section 7 contains a discussion of the results.

2. SOURCES OF ERROR IN SCIENTIFIC COMPUTATION

There are three sources of error that must be considered in scientific computation [7]:

(1) errors due to discretisation and truncation,
(2) errors due to roundoff, and
(3) errors due to uncertainty in the data.

The errors due to discretisation and truncation will not be considered because this paper does not discuss algorithmic issues; interest is restricted to two error models of the perturbations in the polynomial coefficients and their effect on the numerical condition of a root.

Computer hardware can only represent a discrete subset of the real numbers, and the elements in this subset are called floating point numbers. The error that arises from the representation of real numbers by members of this subset is called the roundoff error, and it is usually assumed that it can be represented by a random variable that has a uniform distribution, the bounds of which are $\pm 2^{-53}$ for double precision. Thus each coefficient a_i of a polynomial is perturbed to $a_i + \delta a_i = a_i(1 + r_i\varepsilon_c)$, where r_i is a random number that is uniformly distributed in the interval $[-1, +1]$, and ε_c is the relative roundoff error. It follows that

$$\frac{|\delta a_i|}{|a_i|} \leq \varepsilon_c, \qquad i = 0, \dots, n. \tag{1}$$

Although this model of roundoff error is frequently used, some of the assumptions implicit in it are not satisfied [8,9]. In particular, it is often assumed that roundoff errors are random, weakly correlated, and distributed continuously over a very small interval, but they are not random, they are often correlated, and they frequently behave more like discrete than continuous random variables.

The error model (1) is inappropriate for experimental inaccuracies because numerous scientific measurements have been shown to have a Gaussian distribution [10,11]. In most circumstances, the coefficients of a polynomial are nonlinear functions of the experimental data, and thus they are not independent random variables. A detailed analysis requires that these nonlinear functions be used to calculate the probability density function of the coefficients. However, this is, in general, a very difficult problem, and it is therefore assumed that the effects of measurement and experimental inaccuracies can be quantified by assuming that the coefficients are independent Gaussian random variables.

The boundaries of uncertainty in data are rarely sharply defined, and thus the error model (1) is not representative of typical data. Moreover, measurement inaccuracies are usually significantly more important than are the effects of roundoff error [12]. For example, a typical tolerance that can be accommodated in most CNC (computer numerical control) machines is about five microns, and thus assuming that all dimensions are in metres, only the first five decimal places are important. However, since the relative roundoff error for double precision arithmetic on most computers is $\pm 2^{-53} \approx \pm 10^{-16}$, these two sources of error differ by several orders of magnitude. In other applications, for example biological and economic systems, the errors in the polynomial coefficients may be several percent.

Since the applications described in Section 1 involve computations on the coefficients of polynomials, a measure of the stability of a polynomial basis must be defined. Although there exist several different measures of the condition of a polynomial basis [13], it will be defined by the numerical condition of the roots of the polynomial. This measure is particularly appropriate for geometric computations because of the importance of the determination of the roots of a polynomial for this class of problem.

Let x_0 be a root of the polynomial $p(x)$,

$$p(x) = \sum_{i=0}^{n} a_i \phi_i(x), \tag{2}$$

where $\phi(x) = \{\phi_i(x)\}_{i=0}^{n}$ is a set of linearly independent basis functions that span the space of polynomials of degree n, and a_i is the coefficient (assumed to be real) of the function $\phi_i(x)$. The sensitivity of x_0 is a measure of the numerical condition of x_0 when each coefficient of $p(x)$ is perturbed by an independent zero mean Gaussian random variable. It follows that the perturbations

$\delta a = \{\delta a_i\}_{i=0}^{n}$ satisfy

$$E\{\delta a_i\} = 0, \qquad i = 0, \dots, n, \tag{3}$$

$$E\{\delta a_i \delta a_j\} = \sigma_a^2 \delta_{ij}, \qquad i, j = 0, \dots, n, \tag{4}$$

where E is the expectation operator, δ_{ij} is the two-dimensional delta function, and σ_a^2 is the variance of the perturbations δa_i.

The normwise sensitivity is defined as

$$\rho_p(x_0) = \frac{E\{\Delta x_0\}}{E\{\Delta a_p\}}, \qquad p = 1, 2, \tag{5}$$

and the componentwise sensitivity is defined as

$$\gamma(x_0) = \frac{E\{\Delta x_0\}}{E\{\Delta a_c\}}, \tag{6}$$

where the perturbations δa_i satisfy (3) and (4),

$$\Delta x_0 = \frac{|\delta x_0|}{|x_0|}, \quad \Delta a_p = \frac{\|\delta a\|_p}{\|a\|_p}, \qquad p = 1, 2, \tag{7}$$

and

$$\Delta a_c = \frac{|\delta a_0|}{|a_0|} + \frac{|\delta a_1|}{|a_1|} + \cdots + \frac{|\delta a_n|}{|a_n|}. \tag{8}$$

It follows from (5) and (6) that the sensitivity can be considered an average case measure of condition since expected values are used. This is emphasized by defining the average case measure as the sensitivity and reserving the condition number for its usual definition as a worst case measure.

Definitions (5) and (6) contain the expectation operator E, and this must be compared with definition (1) that leads to a condition number, that is, an upper bound for the displacement of a root. This difference arises because of the fundamentally different nature of the underlying probability density function of the error models (1), and (3) and (4). In particular, the random variables δa_i in (1) are limited to $[-1, +1]$, and thus an upper bound on the displacement of a root can be calculated. However, since these random variables have infinite support in (3) and (4), an upper bound on $|\delta a_i|$ that is analogous to (1) cannot be defined, and the expected value of the displacement of a root is a suitable alternative that is easily calculated.

3. THE NUMERICAL CONDITION OF A ROOT

Expressions for the sensitivity and condition number of a root x_0 of the polynomial (2) are developed in this section. Although the main emphasis is on the sensitivity, expressions for the condition number are included in order to compare average case and worst case measures.

3.1. Average Case Measures of Condition

Expressions for the sensitivity of a root of a polynomial are developed in Theorems 3.1 and 3.2.

THEOREM 3.1. *Let each coefficient a_i of $p(x)$ in (2) be perturbed to $a_i + \delta a_i$ where the perturbations satisfy (3) and (4). Let the real root x_0 of $p(x)$ have multiplicity m, and let one of these m roots be perturbed to $x_0 + \delta x_0$ due to the perturbations in the coefficients. The componentwise sensitivity of x_0 is*

$$\gamma(x_0) = \frac{E\{\Delta x_0\}}{E\{\Delta a_c\}} = \left|\frac{m!}{p^{(m)}(x_0)}\right|^{1/m} \frac{\Pi_1(m)\,\|\phi(x_0)\|_2^{1/m}}{|x_0|\,\|a^{-1}\|_1}, \tag{9}$$

and the normwise sensitivity of x_0 in the 1-norm is

$$\rho_1(x_0) = \frac{E\{\Delta x_0\}}{E\{\Delta a_1\}} = \left|\frac{m!}{p^{(m)}(x_0)}\right|^{1/m} \frac{\Pi_1(m)\,\|\phi(x_0)\|_2^{1/m}\,\|a\|_1}{|x_0|\,(n+1)}, \tag{10}$$

where Δx_0 and Δa_1 are defined in (7), Δa_c is defined in (8),

$$\Pi_1(m) = \left(\sqrt{2}\sigma_a\right)^{(1/m-1)} \Gamma\left(\frac{1}{2}\left(\frac{1}{m}+1\right)\right), \tag{11}$$

and $\Gamma(t)$ is the gamma function,

$$\Gamma(t) = \int_0^{\infty} z^{(t-1)} \exp(-z)\,\mathrm{dz}.$$

PROOF. It is noted that although x_0 is assumed to be real, it does not follow that the perturbed root $x_0 + \delta x_0$ is also real. Furthermore, the perturbed root $x_0 + \delta x_0$ is not, in general, of multiplicity m. The polynomial $p(x^*)$ evaluated at $x^* = x + \delta x$ is

$$\begin{aligned} p(x+\delta x) &= \sum_{i=0}^{n} a_i \phi_i(x+\delta x) \\ &= \sum_{i=0}^{n} (a_i + \delta a_i)\,\phi_i(x+\delta x) - \sum_{i=0}^{n} \delta a_i \phi_i(x+\delta x). \end{aligned}$$

Since $x_0 + \delta x_0$ is a root of the perturbed polynomial, it follows that

$$p(x_0+\delta x_0) = -\sum_{i=0}^{n} \delta a_i \phi_i(x_0+\delta x_0).$$

By Taylor's theorem,

$$p(x_0+\delta x_0) = \sum_{k=0}^{n} p^{(k)}(x_0)\,\frac{(\delta x_0)^k}{k!}$$

and

$$\phi_i(x_0+\delta x_0) = \sum_{k=0}^{n} \phi_i^{(k)}(x_0)\,\frac{(\delta x_0)^k}{k!},$$

and hence

$$\sum_{k=0}^{n} p^{(k)}(x_0)\,\frac{(\delta x_0)^k}{k!} = -\sum_{i=0}^{n} \delta a_i \sum_{k=0}^{n} \phi_i^{(k)}(x_0)\,\frac{(\delta x_0)^k}{k!}. \tag{12}$$

If the perturbation δx_0 is small, only the term of lowest degree on the left-hand side need be considered, and since x_0 has multiplicity m,

$$\begin{aligned} -p^{(m)}(x_0)\,\frac{(\delta x_0)^m}{m!} &\approx \sum_{i=0}^{n} \delta a_i \sum_{k=0}^{n} \phi_i^{(k)}(x_0)\,\frac{(\delta x_0)^k}{k!} \\ &= \sum_{i=0}^{n} \delta a_i \phi_i(x_0) + \delta x_0 \sum_{i=0}^{n} \delta a_i \phi_i^{(1)}(x_0) \\ &\quad + \frac{(\delta x_0)^2}{2!} \sum_{i=0}^{n} \delta a_i \phi_i^{(2)}(x_0) \\ &\quad + \cdots + \frac{(\delta x_0)^n}{n!} \sum_{i=0}^{n} \delta a_i \phi_i^{(n)}(x_0). \end{aligned} \tag{13}$$

Since the perturbations δa_i are random variables, interest is restricted to the expected value, rather than the exact value, of the terms on the right-hand side of (12) and (13). Furthermore, since δx_0 is small, only the term of lowest degree need be considered when calculating the expected value of (12), and thus

$$E\{|\delta x_0|\} = \left|\frac{m!}{p^{(m)}(x_0)}\right|^{1/m} E\left\{\left|\sum_{i=0}^{n} \delta a_i \phi_i(x_0)\right|^{1/m}\right\}. \tag{14}$$

Since δa_i is a random variable, it is necessary to derive the probability density function of the term on the right-hand side of (14). It follows from (3) and (4) that the random variable

$$y = y(x_0) = \sum_{i=0}^{n} \delta a_i \phi_i(x_0)$$

is a zero mean Gaussian random variable with variance

$$\sigma_y^2 = \sigma_a^2 \sum_{i=0}^{n} \phi_i^2(x_0). \tag{15}$$

The probability density function of the random variable

$$z = |y| = \left|\sum_{i=0}^{n} \delta a_i \phi_i(x_0)\right|$$

is

$$f(z) = \frac{1}{\sigma_y}\sqrt{\frac{2}{\pi}} \exp\left(-\frac{z^2}{2\sigma_y^2}\right), \qquad z \geq 0.$$

It follows from (14) that the expected value of the random variable $h = z^{1/m}$ must be computed. If m is even, the solution of the equation $h = z_1^{1/m}$, where z_1 is a given value of z, is $h = \pm(z_1^{1/m})$. However, if m is odd there is only one solution, given by $h = +(z_1^{1/m})$. The probability density function of h is

$$f(h) = \frac{m}{\sigma_y}\sqrt{\frac{2}{\pi}} h^{m-1} \exp\left(-\frac{h^{2m}}{2\sigma_y^2}\right), \qquad h = \left|\sum_{i=0}^{n} \delta a_i \phi_i(x_0)\right|^{1/m} \geq 0,$$

and its expected value is

$$E\{h\} = \frac{m}{\sigma_y}\sqrt{\frac{2}{\pi}} \int_0^\infty h^m \exp\left(-\frac{h^{2m}}{2\sigma_y^2}\right) \mathrm{dh}.$$

The substitution $t = h^{2m}/2\sigma_y^2$ yields

$$E\{h\} = \frac{\left(\sqrt{2}\sigma_y\right)^{1/m}}{\sqrt{\pi}} \int_0^\infty t^{1/2(1/m-1)} \exp(-t)\,\mathrm{dt} = \frac{\left(\sqrt{2}\sigma_y\right)^{1/m}}{\sqrt{\pi}} \Gamma\left(\frac{1}{2}\left(\frac{1}{m}+1\right)\right),$$

and it follows from (11), (14), and (15) that

$$E\{\Delta x_0\} = \frac{1}{|x_0|}\left|\frac{m!}{p^{(m)}(x_0)}\right|^{1/m} \frac{\left(\sqrt{2}\sigma_a\right)^{1/m} \|\phi(x_0)\|_2^{1/m} \Gamma\left((1/2)\,(1/m+1)\right)}{\sqrt{\pi}}. \tag{16}$$

The probability density function of the random variable $\mu_i = |\delta a_i|$ is

$$f(\mu_i) = \frac{1}{\sigma_a}\sqrt{\frac{2}{\pi}}\exp\left(-\frac{\mu_i^2}{2\sigma_a^2}\right), \qquad \mu_i \geq 0,$$

and its expected value is

$$E\{|\delta a_i|\} = \sigma_a\sqrt{\frac{2}{\pi}}.$$

It follows from (8) that the expected value of the relative error in the coefficients for the componentwise measure is

$$E\{\Delta a_c\} = \sigma_a\sqrt{\frac{2}{\pi}}\left\|a^{-1}\right\|_1, \tag{17}$$

and the componentwise sensitivity (9) follows from (16) and (17). The expected value of the relative error in the coefficients for the normwise measure is

$$E\{\Delta a_1\} = \frac{E\left\{\sum\limits_{i=0}^{n}|\delta a_i|\right\}}{\|a\|_1} = \frac{\sum\limits_{i=0}^{n}E\{|\delta a_i|\}}{\|a\|_1} = \sigma_a\sqrt{\frac{2}{\pi}}\frac{(n+1)}{\|a\|_1}, \tag{18}$$

and expression (10) for $\rho_1(x_0)$ follows from (16) and (18). ∎

THEOREM 3.2. *Let each coefficient a_i of $p(x)$ in (2) be perturbed to $a_i + \delta a_i$ where the perturbations satisfy (3) and (4). Let the real root x_0 of $p(x)$ have multiplicity m, and let one of these m roots be perturbed to $x_0 + \delta x_0$ due to the perturbations in the coefficients. The normwise sensitivity in the 2-norm is*

$$\rho_2(x_0) = \sqrt{\frac{E\left\{(\Delta x_0)^2\right\}}{E\left\{(\Delta a_2)^2\right\}}} = \left|\frac{m!}{p^{(m)}(x_0)}\right|^{1/m} \cdot \frac{\Pi_2(m)\,\|\phi(x_0)\|_2^{1/m}\,\|a\|_2}{|x_0|\sqrt{n+1}}, \tag{19}$$

where Δx_0 and Δa_2 are defined in (7), and

$$\Pi_2(m) = \frac{2^{1/2m}\sigma_a^{(1/m-1)}}{\pi^{1/4}}\sqrt{\Gamma\left(\frac{1}{m}+\frac{1}{2}\right)}.$$

PROOF. The proof is similar to that of Theorem 3.1, but (14) is replaced by

$$E\left\{|\delta x_0|^2\right\} = \left|\frac{m!}{p^{(m)}(x_0)}\right|^{2/m} E\left\{\left|\sum_{i=0}^{n}\delta a_i\phi_i(x_0)\right|^{2/m}\right\}.$$

The probability density function of the random variable g, defined by

$$g = h^2 = \left|\sum_{i=0}^{n}\delta a_i\phi_i(x_0)\right|^{2/m},$$

is

$$f(g) = \frac{m}{\sigma_y}\frac{1}{\sqrt{2\pi}}g^{m/2-1}\exp\left(-\frac{g^m}{2\sigma_y^2}\right),$$

and its expected value is

$$E\{g\} = \frac{\left(2\sigma_y^2\right)^{1/m}}{\sqrt{\pi}}\Gamma\left(\frac{1}{m}+\frac{1}{2}\right).$$

It follows that

$$E\left\{|\delta x_0|^2\right\} = \left|\frac{m!}{p^{(m)}(x_0)}\right|^{2/m} \frac{\sigma_a^{2/m} 2^{1/m} \|\phi(x_0)\|_2^{2/m} \Gamma(1/m+1/2)}{\sqrt{\pi}}.$$

The expected value of the square of the relative error in the coefficients is

$$E\left\{(\Delta a_2)^2\right\} = \frac{E\left\{\sum_{i=0}^{n} \delta a_i^2\right\}}{\|a\|_2^2} = \frac{(n+1)\sigma_a^2}{\|a\|_2^2},$$

and result (19) follows. ∎

The substitutions $a_i \to s a_i$, $\delta a_i \to s\delta a_i$, and (from (4)) $\sigma_a^2 \to s^2\sigma_a^2$ do not alter the expressions for $\gamma(x_0)$, $\rho_1(x_0)$, and $\rho_2(x_0)$, thus showing that the sensitivity is dimensionally correct. However, a constant shift t in all the roots (obtained by the substitution $x = z - t$ in $p(x)$) changes the sensitivity of the roots. Since σ_a approaches zero more rapidly than does $\sigma_a^{1/m}$ for $m > 1$, it follows that $\gamma(x_0), \rho_1(x_0), \rho_2(x_0) \to \infty$ as $\sigma_a \to 0$ for multiple roots. This point will be considered in further detail in Section 4, where it will be shown that it explains the inherently ill-conditioned nature of multiple roots.

3.2. Worst Case Measures of Condition

Expressions for the componentwise and normwise condition numbers of x_0 are stated in the following theorem. The proofs are in [14].

THEOREM 3.3. *Let each coefficient a_i of $p(x)$ be perturbed to $a_i + \delta a_i$, and let the real root x_0 of $p(x)$ have multiplicity m. If one of these m roots is perturbed to $x_0 + \delta x_0$ due to the perturbations in the coefficients, then the componentwise condition number of x_0 is*

$$\chi(x_0) = \frac{1}{\varepsilon_c^{1-1/m} |x_0|} \left(\frac{m! \sum_{i=0}^{n} |a_i \phi_i(x_0)|}{|p^{(m)}(x_0)|} \right)^{1/m}, \tag{20}$$

and the normwise condition number of x_0 is

$$\psi(x_0) = \frac{1}{\varepsilon_n^{1-1/m} |x_0|} \left(\frac{m! \|a\|_2 \|\phi(x_0)\|_2}{|p^{(m)}(x_0)|} \right)^{1/m}, \tag{21}$$

where ε_c is defined in (1), and

$$\|\delta a\|_2 \le \varepsilon_n \|a\|_2.$$

There is one more point that must be considered in the derivations of the expressions for the sensitivities and condition numbers. In particular, the left-hand side of (13) follows from the left-hand side of (12) if

$$\frac{\left|p^{(m+1)}(x_0)(\delta x_0)^{m+1}\right|}{(m+1)!} \ll \frac{\left|p^{(m)}(x_0)(\delta x_0)^m\right|}{m!}$$

or

$$|\delta x_0| \ll \frac{(m+1)\left|p^{(m)}(x_0)\right|}{\left|p^{(m+1)}(x_0)\right|}. \tag{22}$$

If x_0 is well removed from its nearest neighbouring root, this equation is easily satisfied. However, if there exists a root that is near x_0, caution must be exercised because condition (22) may place tight restrictions on the forward error δx_0. The difficulties that arise, in both condition estimation and backward error analysis, when (22) is not satisfied are considered in [15].

EXAMPLE 3.1. Consider the polynomial

$$p(x) = (x - x_0)^2 (x - x_0 - \epsilon).$$

For the double root x_0, condition (22) becomes $|\delta x_0| \ll |\epsilon|$, and thus the forward error must be significantly smaller than the root separation. This condition is easily satisfied if $|\epsilon|$ is large, but if ϵ is small such that x_0 is almost a triple root, (22) may not be satisfied. ∎

It will be assumed throughout that the root x_0 is well separated from its nearest neighbouring root, such that (22) is always satisfied.

4. THE CAUSE OF ILL-CONDITIONED ROOTS

The results developed in the previous section are used to determine the cause of ill-conditioning of multiple roots. The situation for simple roots is considered by Demmel [16], who shows that the distance to the nearest polynomial in which a simple root y_0 merges into a double root is bounded by a small multiple of the reciprocal of the condition number of y_0.

In order to investigate the cause of ill-conditioning of a multiple root x_0, it is assumed that $|x_0| \gg 0$ and x_0 is sufficiently far from its nearest root, as noted in Example 3.1. It is convenient to write expression (10) for $\rho_1(x_0)$ in the form

$$\Theta(m) \frac{\|\phi(x_0)\|_2^{1/m}}{|x_0|} \frac{\|a\|_1^{1/m}}{\left|p^{(m)}(x_0)\right|^{1/m}} \frac{\|a\|_1^{(1-1/m)}}{\sigma_a^{(1-1/m)}(n+1)},$$

where

$$\Theta(m) = (m!)^{1/m} 2^{(1/2)(1/m-1)} \Gamma\left(\frac{1}{2}\left(\frac{1}{m}+1\right)\right).$$

The function $\Theta(m)$ is shown in Figure 1 and it is seen that even for large values of m, this expression increases approximately linearly with m, such that this term is not the source of the

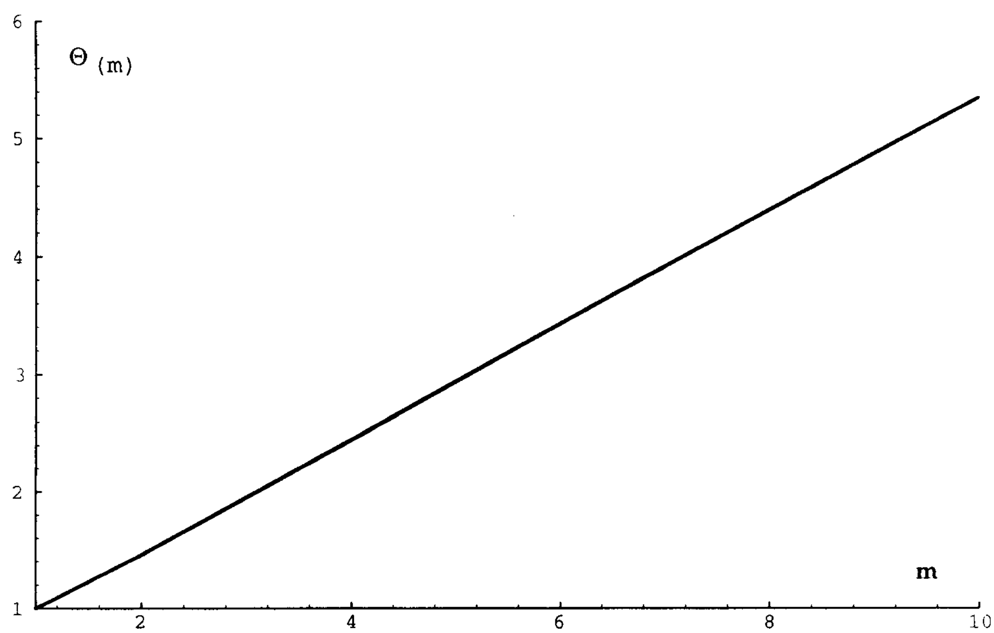

Figure 1. The function $\Theta(m)$ against m.

ill-conditioned nature of multiple roots. The almost linear variation of $\Theta(m)$ with large values of m follows from Stirling's approximation for the factorial function and the replacement of the gamma function by a constant,

$$m! \approx \sqrt{2\pi m}\exp(-m)m^m \qquad \text{and} \qquad \Gamma\left(\frac{1}{2}\left(\frac{1}{m}+1\right)\right) \approx \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi},$$

respectively. Thus, if $m \gg 1$,

$$\Theta(m) \approx 2^{(1/m-1/2)}\pi^{(1/2)\,(1/m+1)}m^{(1+1/2m)}\exp\left(-1\right) \approx \sqrt{\frac{\pi}{2}}\exp\left(-1\right)m,$$

and hence the variation of $\Theta(m)$ with large values of m is approximately linear. It is readily checked that the error between the gradient of this linear approximation and the gradient of the curve in Figure 1 is small, and it is seen that this approximation is good, even for small values of m. Since it is assumed that x_0 is well separated from its nearest root and $|x_0| \gg 0$, the functions

$$\frac{\|\phi\left(x_0\right)\|_2^{1/m}}{|x_0|} \qquad \text{and} \qquad \frac{\|a\|_1^{1/m}}{\left|p^{(m)}\left(x_0\right)\right|^{1/m}}$$

are not large, and it follows that the order of magnitude of $\rho_1(x_0)$ is governed by the term

$$\frac{1}{n+1}\left(\frac{\|a\|_1}{\sigma_a}\right)^{1-1/m}.$$

Since

$$\sigma_a^2 \approx \frac{\|\delta a\|_2^2}{n+1}, \tag{23}$$

it follows that

$$\frac{1}{n+1}\left(\frac{\|a\|_1}{\sigma_a}\right)^{1-1/m} \approx \frac{1}{(n+1)^{(1/2)\,(1+1/m)}}\left(\frac{\|a\|_1}{\|\delta a\|_2}\right)^{1-1/m},$$

and hence the order of magnitude of $\rho_1(x_0)$ is governed by the ratio of the 1-norm of the coefficients to the 2-norm of the perturbations in the coefficients.

Consideration of (19) shows that the dominant term in the expression for $\rho_2(x_0)$ is

$$\frac{1}{\sqrt{n+1}}\left(\frac{\|a\|_2}{\sigma_a}\right)^{1-1/m},$$

and (23) enables this expression to be simplified. Similar analysis can be carried out for the condition numbers $\chi(x_0)$ and $\psi(x_0)$, and it is concluded for all the measures that a multiple root becomes more sensitive to the effects of perturbations in the coefficients as the signal-to-noise ratio increases, and it is therefore difficult to compute multiple roots reliably even when the data have little noise. Furthermore, if a polynomial $p(x)$ that has a multiple root is expressed in two different bases, and the signal-to-noise ratio is approximately constant, then the numerical condition (as measured by the condition number or sensitivity) of the multiple root is weakly dependent on the basis of $p(x)$.

5. COMPONENTWISE AND NORMWISE MEASURES

It is shown that the distinction between the componentwise and normwise definitions of the sensitivity and condition numbers is important because they yield condition estimates that may differ by several orders of magnitude, depending upon the coefficients of the polynomial.

Consider first the sensitivity. It follows from (9) and (10) that

$$\rho_1\left(x_0\right) = \gamma\left(x_0\right)\frac{\|a\|_1\left\|a^{-1}\right\|_1}{(n+1)}. \tag{24}$$

The equivalent result for the ratio of the normwise condition number $\psi(x_0)$ to the componentwise condition number $\chi(x_0)$ is derived in the following theorem.

THEOREM 5.1. *Upper and lower bounds for the ratio of* $\psi(x_0)$ *to* $\chi(x_0)$ *are, respectively,*

$$\frac{\psi(x_0)}{\chi(x_0)} \le \left(\frac{\varepsilon_c}{\varepsilon_n}\right)^{1-1/m} \left(\left\|a^{-1}\right\|_\infty \|a\|_2 \frac{\|a \circ \phi(x_0)\|_2}{\|a \circ \phi(x_0)\|_1}\right)^{1/m} \tag{25}$$

and

$$\frac{\psi(x_0)}{\chi(x_0)} \ge \left(\frac{\varepsilon_c}{\varepsilon_n}\right)^{1-1/m} \left(\|a\|_\infty^{-1} \|a\|_2 \frac{\|a \circ \phi(x_0)\|_2}{\|a \circ \phi(x_0)\|_1}\right)^{1/m}, \tag{26}$$

where $a \circ \phi(x_0) = \{a_i \phi_i(x_0)\}_{i=0}^n$ *is the Hadamard (Schur) product of* a *and* $\phi(x_0)$.

PROOF. Consider first the upper bound. Since

$$\begin{aligned}
\frac{\|\phi(x_0)\|_2 \|a\|_2}{\sum_{i=0}^n |a_i \phi_i(x_0)|} &= \frac{\sqrt{\sum_{i=0}^n (1/a_i^2)\, a_i^2 \phi_i^2(x_0)}\|a\|_2}{\sum_{i=0}^n |a_i \phi_i(x_0)|} \\
&\le \frac{\max\{1/|a_i|\} \sqrt{\sum_{i=0}^n a_i^2 \phi_i^2(x_0)}\|a\|_2}{\sum_{i=0}^n |a_i \phi_i(x_0)|} \\
&= \frac{\left\|a^{-1}\right\|_\infty \|a\|_2 \|a \circ \phi(x_0)\|_2}{\|a \circ \phi(x_0)\|_1},
\end{aligned}$$

the upper bound (25) follows from (20) and (21).

Consider now the lower bound,

$$\begin{aligned}
\frac{\|\phi(x_0)\|_2 \|a\|_2}{\sum_{i=0}^n |a_i \phi_i(x_0)|} &= \frac{\sqrt{\sum_{i=0}^n (1/a_i^2)\, a_i^2 \phi_i^2(x_0)}\|a\|_2}{\sum_{i=0}^n |a_i \phi_i(x_0)|} \\
&\ge \frac{\min\{1/|a_i|\} \sqrt{\sum_{i=0}^n a_i^2 \phi_i^2(x_0)}\|a\|_2}{\sum_{i=0}^n |a_i \phi_i(x_0)|} \\
&= \frac{\|a\|_2 \|a \circ \phi(x_0)\|_2}{\max\{|a_i|\} \sum_{i=0}^n |a_i \phi_i(x_0)|} \\
&= \frac{\|a\|_\infty^{-1} \|a\|_2 \|a \circ \phi(x_0)\|_2}{\|a \circ \phi(x_0)\|_1},
\end{aligned}$$

and result (26) follows from (20) and (21). ∎

Equation (24) for the sensitivities, and (25) and (26) for the condition numbers, have both similarities and differences. In particular, the ratio of the upper bound (25) to the lower bound (26) for a simple root is equal to $\|a^{-1}\|_\infty \|a\|_\infty$, and (24) shows that an identical term (apart from the difference in the norm and the factor $(n+1)^{-1}$) is valid for the sensitivities. Thus, if the coefficients a_i differ by several orders of magnitude, the condition numbers and sensitivities of a simple root also vary greatly in magnitude. However, if m is large, then

$$\frac{\psi(x_0)}{\chi(x_0)} \approx \frac{\varepsilon_c}{\varepsilon_n},$$

because the second term on the right-hand side of (25) and (26) is approximately one. It follows that the ratio of the normwise condition number to the componentwise condition number of a high degree multiple root is approximately independent of the basis functions and only a function of ε_c and ε_n, where ε_c^{-1} and ε_n^{-1} are measures of the componentwise and normwise signal-to-noise ratios. This result is consistent with the results in Section 4.

An important difference between (24), and (25) and (26), arises from their dependence on the multiplicity m. Specifically, it appears explicitly in (25) and (26) through the exponents of the terms, and implicitly through the constraints that a multiple root imposes on the coefficients a_i. However, m only enters implicitly in (24) for the normwise and componentwise sensitivities.

6. EXAMPLES

This section contains three examples that demonstrate the theory presented in the previous sections. The x-axes in all the graphs in this section are the roots of a polynomial and the y-axes are the computed and/or theoretical values of their condition numbers and/or sensitivities.

EXAMPLE 6.1. Consider the Wilkinson polynomial

$$p(x) = \prod_{i=1}^{20} \left(x - \frac{i}{20} \right) = \sum_{i=0}^{20} a_i x^i, \tag{27}$$

whose roots are $x_i = i/20$, $i = 1, \ldots, 20$. The effects of a perturbation in only one coefficient are investigated in [17,18], and it is shown that the roots of this polynomial are ill-conditioned. However, all the coefficients are perturbed in this example.

Polynomial (27) was generated and each coefficient was perturbed by an independent zero mean Gaussian random variable of standard deviation $\sigma_a = 10^{-14}$. The roots of the perturbed polynomial were computed and the componentwise and normwise sensitivities of each root were calculated by noting the change δx_i in each root x_i, thus enabling the relative change $\Delta x_i = |\delta x_i|/x_i$ to be determined. The experiment was repeated four times and the average value of these sensitivities of each root over the five trials was calculated. The results are plotted in Figure 2 for the 1-norm; the results for the 2-norm are very similar and are not shown. It is seen that there is excellent agreement between the computed and theoretical sensitivities, and that the ratio of the normwise sensitivity to the componentwise sensitivity is about 10^{10}. This figure is in agreement with (24) because $\|a\|_1 = 3.20 \times 10^3$ and $\|a^{-1}\|_1 = 4.37 \times 10^7$. Excellent agreement was also obtained between the theoretical and computed values of the sensitivity $\rho_2(x_i)$.

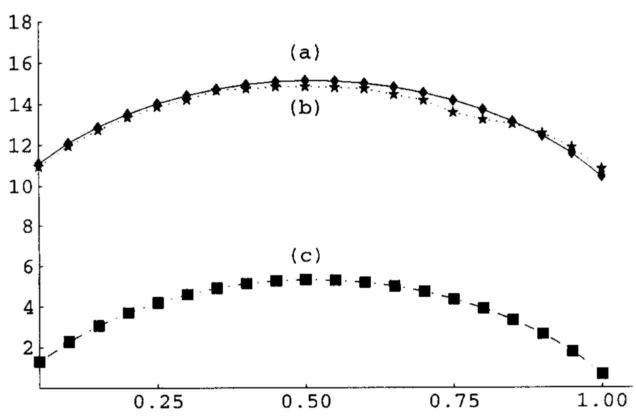

Figure 2. The logarithm to base 10 of (a) solid line, the theoretical value of the normwise sensitivity in the 1-norm $\rho_1(x_i)$, (b) dashed line, the computed value of $\rho_1(x_i)$, and (c) the componentwise sensitivity $\gamma(x_i)$, with $x_i = i/20$, $i = 1, \ldots, 20$, for Example 6.1.

Figure 3 shows the componentwise and normwise condition numbers, $\chi(x_i)$ and $\psi(x_i)$, respectively. It is seen that the ratio of the normwise condition number to the componentwise condition number is about 10^{10} for the small roots, and about one for the roots that are near $x_{20} = 1$. This computed figure is in agreement with (25) and (26) because $\|a\|_\infty = 628$ and $\|a^{-1}\|_\infty = 4.31 \times 10^7$. Figure 4 shows the componentwise condition number and sensitivity, $\chi(x_i)$ and $\gamma(x_i)$, respectively, and it is seen that these two measures are approximately equal for the roots near $x_1 = 1/20$, but that they differ by several orders of magnitude for the larger roots. ∎

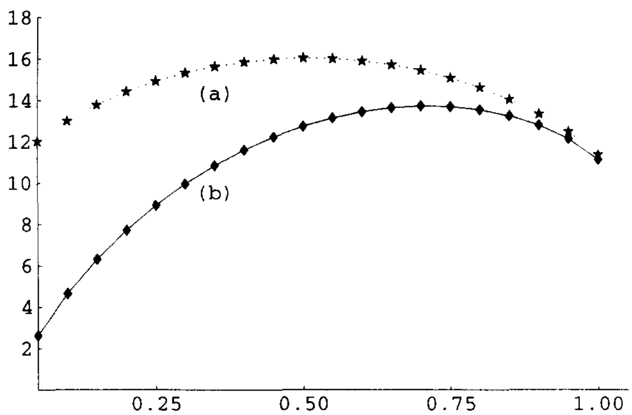

Figure 3. The logarithm to base 10 of (a) the normwise condition number $\psi(x_i)$, and (b) the componentwise condition number $\chi(x_i)$, with $x_i = i/20$, $i = 1, \dots, 20$, for Example 6.1.

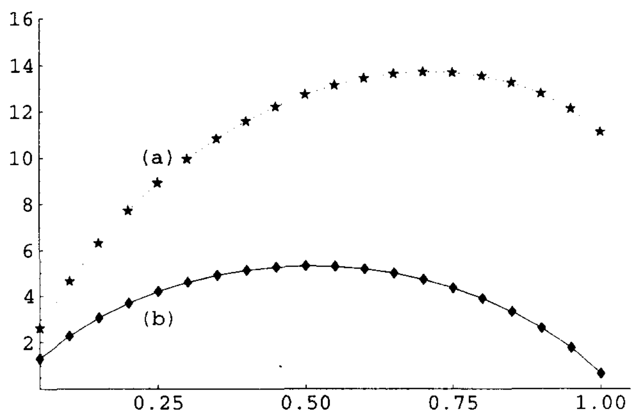

Figure 4. The logarithm to base 10 of (a) the componentwise condition number $\chi(x_i)$, and (b) the componentwise sensitivity $\gamma(x_i)$, with $x_i = i/20$, $i = 1, \dots, 20$, for Example 6.1.

EXAMPLE 6.2. Consider the polynomial

$$p(x) = \prod_{i=1}^{10} \left(x - 2^{-i}\right) = \sum_{i=0}^{10} a_i x^i, \tag{28}$$

whose roots are $x_i = 2^{-i}$, $i = 1, \dots, 10$. The procedure described in Example 6.1 was repeated except that the standard deviation σ_a was changed to 10^{-17}. Figure 5 shows the theoretical and computed values of the normwise sensitivity $\rho_1(x_i)$ and the componentwise sensitivity $\gamma(x_i)$,

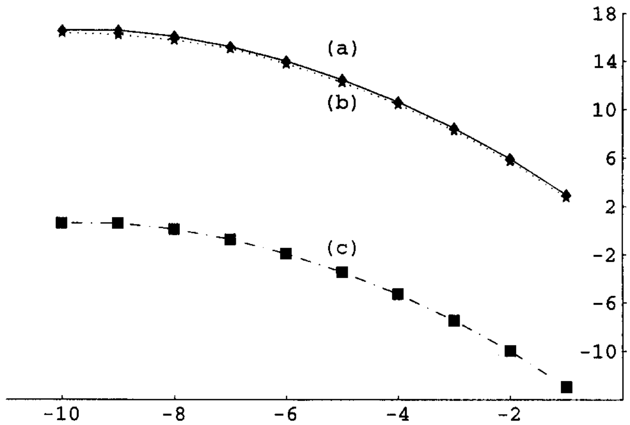

Figure 5. The logarithm to base 10 of (a) solid line, the theoretical value of the normwise sensitivity in the 1-norm $\rho_1(x_i)$, (b) dashed line, the computed value of $\rho_1(x_i)$, and (c) the componentwise sensitivity $\gamma(x_i)$, with $\log_2 x_i = -i$, $i = 1, \ldots, 10$, for Example 6.2.

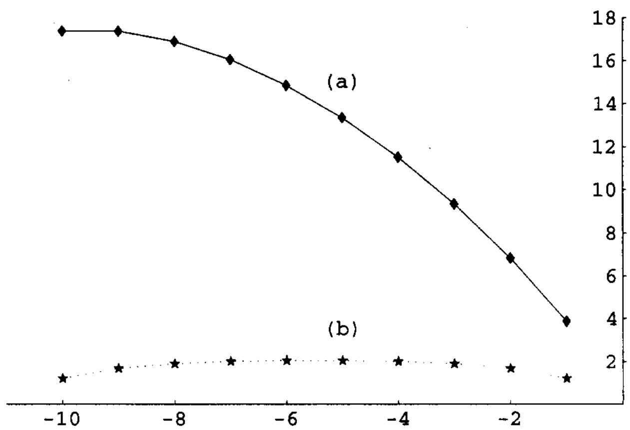

Figure 6. The logarithm to base 10 of (a) the normwise condition number $\psi(x_i)$, and (b) the componentwise condition number $\chi(x_i)$, with $\log_2 x_i = -i$, $i = 1, \ldots, 10$, for Example 6.2.

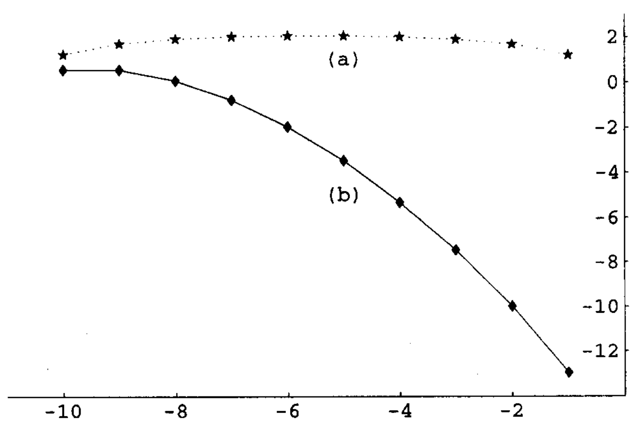

Figure 7. The logarithm to base 10 of (a) the componentwise condition number $\chi(x_i)$, and (b) the componentwise sensitivity $\gamma(x_i)$, with $\log_2 x_i = -i$, $i = 1, \ldots, 10$, for Example 6.2.

Figure 6 shows the normwise and componentwise condition numbers, $\psi(x_i)$ and $\chi(x_i)$, respectively, and Figure 7 shows the componentwise condition number and sensitivity, $\chi(x_i)$ and $\gamma(x_i)$, respectively.

Figure 5 shows that the computed values of $\rho_1(x_i)$ agree with their theoretical values, and that the ratio between $\rho_1(x_i)$ and $\gamma(x_i)$ is about 10^{15}. This value is in agreement with (24) because $\|a^{-1}\|_1 = 3.60 \times 10^{16}$ and $\|a\|_1 = 2.38$. Figure 6 shows that the normwise and componentwise condition numbers differ by several orders of magnitude for nearly all the roots, and that the minimum ratio occurs for the largest root $x_1 = 1/2$. However, Figure 7 shows that the componentwise condition number $\chi(x_i)$ is approximately equal to the componentwise sensitivity $\gamma(x_i)$ for the smallest root $x_{10} = 2^{-10}$, but that the ratio between these two measures increases rapidly as the root x_i increases. ∎

EXAMPLE 6.3. Consider the polynomial

$$p(x) = \left(x - \frac{1}{2}\right)^{10} = \sum_{i=0}^{10} a_i x^i. \tag{29}$$

An independent zero mean Gaussian random number of standard deviation $\sigma_a = 10^{-6}$ was added to each coefficient and the sensitivity of the root $x_0 = 1/2$ was calculated experimentally by repeating the procedure described in Example 6.1. The computed values of $\rho_1(1/2)$ and $\rho_2(1/2)$ were, respectively, 2.929×10^6 and 3.538×10^6, which must be compared with the theoretical values, $\rho_1(1/2) = 3.161 \times 10^6$ and $\rho_2(1/2) = 3.641 \times 10^6$.

It was shown in Section 4 that the dominant terms in the expressions for the sensitivity in the 1- and 2-norms are

$$d_1 = \frac{1}{n+1}\left(\frac{\|a\|_1}{\sigma_a}\right)^{1-1/m} \quad \text{and} \quad d_2 = \frac{1}{\sqrt{n+1}}\left(\frac{\|a\|_2}{\sigma_a}\right)^{1-1/m},$$

respectively. Since the 1- and 2-norms of the coefficients are 57.665 and 24.970, respectively, it follows that $d_1 = 8.779 \times 10^5$ and $d_2 = 1.371 \times 10^6$, and thus the signal-to-noise ratio of the coefficients is a good approximation to the sensitivity for both norms, as expected. ∎

7. DISCUSSION

Several different measures of the numerical stability of a root of a polynomial have been considered, and it has been shown that they may be defined in either a componentwise or a normwise sense, and in either a worst case or average case sense. These distinctions are important because two different measures of the stability of a root may differ by several orders of magnitude. For example, Figures 2 and 3 show that the condition number $\chi(x_0)$ for polynomial (27) shows a much greater variation in magnitude than does the sensitivity $\rho_1(x_0)$, but the opposite characteristic is observed for polynomial (28)—Figures 5 and 6 show that the condition number $\chi(x_0)$ is almost constant but $\rho_1(x_0)$ varies by about 13 orders of magnitude. These results illustrate the results in Section 5 because the coefficients of the polynomials in these examples vary greatly in magnitude. Specifically, the coefficients of polynomial (27) range in magnitude from $a_0 = 2.32 \times 10^{-8}$ to $a_{20} = 1$, and the coefficients of polynomial (28) range in magnitude from $a_0 = 2.78 \times 10^{-17}$ to $a_{10} = 1$. The results for polynomial (29) agree with the theoretical predictions because the signal-to-noise ratio is a good approximation to both the sensitivity and condition number.

It was noted in Section 1 that an average case measure of stability is a more practical guide to the numerical condition of a root of a polynomial because the condition number may overestimate the average value by several orders of magnitude. This is clearly evident in Figures 4 and 7, which show that the componentwise sensitivity and condition number for a given polynomial may be approximately equal for some roots of a polynomial, but differ by several orders of magnitude for other roots of the polynomial. From a strictly mathematical consideration, the sensitivity and condition number differ in the probabilistic nature of the underlying error model; the former is defined by the Gaussian model (3) and (4), and the latter is defined (in the componentwise form) by the uniform distribution (1). This shows that the assignment of the correct probabilistic model to an error process is important, and although an incorrect choice will lead to a correct mathematical condition estimate, it will not faithfully represent the correct underlying error process. Furthermore, since the componentwise and normwise condition numbers and sensitivities may differ by several orders of magnitude, the condition measure (average case or worst case, componentwise or normwise) must be defined with care, such that the desired measure is used.

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