Computations in the neighbourhood of algebraic singularities

Françoise Chatelin* **Valérie Fraysse†**
Thierry Braconnier‡

Dedicated to the memory of Farouk Odeh

Abstract

It is known that finite precision versus exact computation is a crucial issue only when the computation takes place in the neighbourhood of a singularity. In such a situation, it is essential to know the distance to singularity. Much attention has been dedicated to the relationship between the distance to singularity δ and the condition number K of the problem under study. The well-known Turing theorem states that, for a linear system $Ax = b$, the distance to singularity, in a normwise measure, is the reciprocal of the normwise condition number $\|A^{-1}\|\|A\|$. In this paper, we examine the possibility of extending this theorem for nonlinear problems in the neighbourhood of algebraic singularities. After reviewing the literature on that topic (Demmel (1987, 1990), Shub and Smale (1992)), we propose and check on the computer a conjecture which makes more explicit Demmel's asymptotic bounds on the distance to singularity.

1 Survey of finite precision computation

We consider the mathematical problem

$$(P) \quad F(x) = y \tag{1}$$

for which we assume there is a locally unique solution $x = F^{-1}(y)$, that we wish to compute. F is a map, nonlinear in general, from X to Y, which are, for instance,

*Laboratoire Central de Recherche, Thomson-CSF, 91404 Orsay Cedex, and University Paris IX Dauphine. Email: chatelin@thomson-lcr.fr

†CERFACS, 42 av. Coriolis, 31057 Toulouse Cedex, France. Email: fraysse@cerfacs.fr

‡CERFACS, 42 av. Coriolis, 31057 Toulouse Cedex, France and ERIN, University of Nancy. Email: braconni@cerfacs.fr

normed vector spaces.

We suppose that F (resp. F^{-1}) is continuous in the neighbourhood of x (resp. y). The problem (P) is then *well-posed* in the sense of Hadamard: the solution x exists, is unique, and F^{-1} is continuous. The continuity of F^{-1} is often referred to as a *stability* property for (P), since a small variation in the datum y induces a small variation in the solution x. The following definition is widespread in mathematics and physics:

Definition 1.1

i) $x = F^{-1}(y)$ *is said to be a* regular *point iff* x *is* C^1 *in the neighbourhood of* y. *Equivalently, one says that the problem* (P) $F(x) = y$ *is regular.*

ii) x *is* singular *whenever it is not regular, that is, when* x *is not* C^1.

In order to investigate the influence of finite precision computation on the accuracy obtained for x, we use the general framework of perturbation theory, as is standard in Numerical Analysis since Wilkinson (1963). In particular, we interpret the computed solution $\tilde{x}$ as the exact solution of a slightly perturbed problem of the same type as (P), that is $(F + \delta F)(\tilde{x}) = y + \delta y$, or equivalently $F(\tilde{x}) = y + \Delta y$.

Definition 1.2 *The solution* x *is said to be* computable *in finite precision arithmetic iff* $\Delta x = \tilde{x} - x$ *tends to* 0 *as the machine precision*[1] *tends to* 0.

In principle, the solution of any well-posed problem is computable using finite precision arithmetic, since a small perturbation Δy in the data of (P) induces a small perturbation Δx in the solution x. But of course, the smoother the solution, the better the accuracy $\|\Delta x\|/\|x\|$, with $\Delta x = \tilde{x} - x$. And the best situation consists of a **regular** problem. In such a case, $\|\Delta x\|$ is proportional to $\|\Delta y\|$ and the sensitivity of x to small changes in y can be measured by a number which is traditionally called the **linear condition number** (denoted K later on) of the problem in Numerical Analysis.
This amounts to a measure of the Fréchet derivative $DF^{-1}(y)$ of F^{-1} at y, with appropriate norms on X and Y (see Rice (1966), Geurts (1982), Chatelin and Frayssé (1992)).

At a singular point, on the contrary, $\|\Delta x\|$ is not proportional to $\|\Delta y\|$ any more, and the linear condition number is either infinite or does not exist. Moreover, singular problems are not generic; under perturbations, such as that induced

[1] The **machine precision** Ψ is defined by $\Psi = 1^+ - 1$ where 1^+ is the successor of 1 in the computer arithmetic. The machine precision Ψ can tend to zero only in theory.

by finite precision arithmetic, singular problems are usually transformed into regular problems which then appear as classically ill-conditioned (their linear condition number tends to be extremely large). In addition, a computation at a regular point which is close enough to a singularity, is driven by the underlying singularity, and results computed with finite precision arithmetic may differ significantly from the exact results.
This viewpoint is not new (Kahan (1972)) and has recently received a lot of attention (Demmel (1987, 1990), Shub and Smale (1992)), especially the relationship between the condition number and the distance to singularity.

In this paper, we intend to take a closer look at various distances of the above kind that can be defined for **nonlinear** problems. We shall focus on a particular class of singularities that we call **algebraic** according to

Definition 1.3 *A singularity is said to be* algebraic *in one of the two following cases:*

i) *(P) is a well-posed problem: x is a* multiple *root of multiplicity m of $F(x) = y$: the successive derivatives of F at x are zero, up to the order $m-1$,*

ii) *(P) is a particular case of an ill-posed problem consisting of a linear system $Ax = b$, when A is singular.*

In case *i)*, $x = F^{-1}(y)$ is not C^1 but at least C^0, while in case *ii)* either x does not exist, or if it exists, it is not unique.

Example 1.1

a) x is a root of multiplicity $m > 1$ of a polynomial $p(x) = 0$, that is $p'(x) = \ldots = p^{(m-1)}(x) = 0$, $p^{(m)}(x) \neq 0$. Then x is Hölder-continuous of order $1/m$.

b) λ is a defective eigenvalue of A of multiplicity m and ascent[2] l, $1 < l \leq m$. Then λ is Hölder-continuous of order $1/l$. If λ is a semi-simple eigenvalue, that is if $l = 1$, then λ is Lipschitz-continuous.

An algebraic singularity which is Hölder-continuous is also called a Hölder-singularity. Clearly, multiple roots define a *hierarchy* of increasing singularity: simple / double / triple / ..., which is a hierarchy of decreasing regularity. Indeed a double root is singular when compared to simple roots (more regular point) but regular when compared to a triple root (more singular point). The notions "regular" / "singular" are context dependant: they depend on the chosen viewpoint.

[2]The *ascent* l is the order of the largest Jordan block associated with λ.

Definition 1.4 *The order γ of a Hölder-continuous regular / singular point is by definition the order of its Hölder-continuity.*

In Example 1.1, $\gamma = 1/m$ in case a) and $\gamma = 1/l$ in case b).

Two remarks are in order before we end this first section:

1. Although in Numerical Analysis one usually refers to "the" condition number of the problem, it is essential to bear in mind that many condition numbers can be associated with one problem. Indeed, the condition number depends on the choice of metrics, the data allowed to be perturbed, the type of admissible perturbations, etc. For example, the condition numbers for $Ax = b$ corresponding to a normwise and a componentwise analysis may differ significantly (Geurts (1982), Chatelin and Frayssé (1992)).

2. In Numerical Linear Algebra, a singular problem is sometimes called "ill-posed" because its classical condition number is infinite (Demmel (1987), Shub and Smale (1992)). In case *i)* of the definition 1.3 above, this terminology would conflict with the fact that the problem is well-posed in the sense of Hadamard. That is why we depart from the Numerical Linear Algebra terminology (ill-posed), to go back to the terminology of singularity more familiar to mathematicians and physicists.

2 On the distance to singularity for linear problems

The problem (P) is taken to be the linear system $Ax = b$. Its normwise relative condition number $K = \|A\|\|A^{-1}\|$ is infinite when the matrix A is singular. The only way to make the system $Ax = b$ singular is to perturb the elements of A. Therefore the only way to define the relative distance to singularity in a normwise analysis (modulo the choice of norms) is

$$\delta = \min\{\omega;\ \|\Delta A\| \le \omega\|A\| \text{ such that } A + \Delta A \text{ is singular}\}.$$

The following theorem is well-known:

Theorem 2.1

$$\delta = \frac{1}{\|A\|\|A^{-1}\|}.$$

This theorem, often attributed to Turing, seems to have already been proved by Banach in the 20s. It was rediscovered by Eckart and Young in 1939 using the 2-norm, and proved by Gastinel for an arbitrary norm. Theorem 2.1 shows that the condition number of a matrix is the reciprocal of the distance to singularity, for a normwise analysis. Yet such a result does not hold for a componentwise analysis. One can exhibit examples for which the reciprocal of the componentwise condition number can be arbitrarily smaller than the componentwise distance to singularity (Rohn (1990), Demmel (1992)). However in our experiments (Chatelin and Frayssé (1993, Chap. 7)), we found that the *distance to singularity viewed by the computer*, which we define later, remains of the order of the reciprocal of the condition number.

How can Theorem 2.1 be extended to **nonlinear** problems? We begin our study by looking at two simple examples.

3 Two simple examples

3.1 The double root of a polynomial

Consider the quadratic polynomial $p(x) = x^2 - 2bx + c$ which has two simple roots $x = b \pm \sqrt{b^2 - c}$, if the discriminant $D = b^2 - c$ is nonzero. The linear condition number K is proportional to the reciprocal of the derivative, that is,

$$K \propto \frac{1}{|p'(x)|} = \frac{1}{2|\sqrt{D}|}.$$

As expected, K is infinite when $D = 0$, that is, when $x = b$ is a double root for p. For $D \neq 0$, the natural question is: can $|\sqrt{D}|$ be considered to be proportional to some appropriately defined distance to singularity of $p(x) = 0$? The answer is yes, if one considers the **constrained** distance to singularity Δ defined as:

$$\Delta = \min\{|\Delta p| \text{ such that } p + \Delta p \text{ has a double root at } x\}.$$

Such a distance is called constrained because only the polynomial p is allowed to vary, whereas the solution x is kept fixed. Let us compute Δp. The simple root $x = b - \sqrt{D}$ of $p(z) = 0$ becomes a double root for $(p+\Delta p)(z) = z^2 - 2(b-\sqrt{D})z + 2b^2 - c - 2b\sqrt{D} = p(z) + 2D - 2b\sqrt{D} - 2z\sqrt{D}$. Therefore, $\Delta p(z) = -2z\sqrt{D} + 2D - 2b\sqrt{D}$. Hence, with the $\|\ .\ \|_\infty$ norm for polynomials, $\Delta = |\Delta p| = \max\left\{|2\sqrt{D}|,\ |2D - 2b\sqrt{D}|\right\}$, which is of the order of $\sqrt{D}$ for D small enough.

But of course, the constrained distance to singularity does not realize the **minimal** distance to singularity δ defined as:

$$\delta = \min\{|\Delta p| \text{ such that } p + \Delta p \text{ has a double root near } x\}.$$

In such a definition, both the polynomial p and its zeroes are allowed to vary. Hence, clearly, $\Delta \geq \delta$.

In the above example, $\delta = |p(x) - (x-b)^2| = |c - b^2| = |D|$. This shows that $\Delta \sim |\sqrt{D}|$ is much larger than $\delta = |D|$, for $|D|$ smaller than 1. Note that δ (resp. Δ) is proportional to $1/K^2$ (resp. $1/K$) when D approaches 0.

3.2 The double defective eigenvalue of a matrix

We now consider the two simple eigenvalues a and b of

$$A = \begin{pmatrix} a & 1 \\ 0 & b \end{pmatrix},$$

for $a \neq b$. The linear condition number for the eigenvalue a is easily computed: $K = \sqrt{1 + 1/(a-b)^2}$. It is infinite when $a = b$ is a double defective eigenvalue. A simple calculation shows that:

i) the constrained distance to singularity $\Delta = |b - a|$ is achieved by

$$\Delta A = \begin{pmatrix} 0 & 0 \\ 0 & a-b \end{pmatrix}:$$

the simple eigenvalue a becomes double.

ii) the minimal distance to singularity $\delta = (a-b)^2/4$ is achieved by

$$\Delta A = \begin{pmatrix} 0 & 0 \\ (a-b)^2/4 & 0 \end{pmatrix}:$$

the nearby eigenvalue $(a+b)/2$ becomes double.

One sees again that δ (resp. Δ) is proportional to $1/K^2$ (resp. $1/K$) when $|b - a|$ tends to 0.

These two trivial examples show that there is no unique answer to the question of how to extend of Theorem 2.1 to nonlinear equations. It is clear that the distinction between Δ and δ vanishes in the case of linear problems, since in that case one has not the option to let x vary because no solution exists at the singularity.

We now review the two approaches in the literature for nonlinear problems taken by the main authors on the subject (Shub and Smale, Demmel).

4 Constrained and minimal distances to singularity for nonlinear problems

Without loss of generality, we can write (P) in the form $F(x) = 0$. The constrained and minimal distances of the problem (P) to singularity are therefore defined as

$$\begin{cases} \Delta = \min\{\|\Delta F\|,\ (F + \Delta F)(x) = 0 \text{ has a multiple root at } x\}, \\ \delta = \min\{\|\Delta F\|,\ (F + \Delta F)(y) = 0 \text{ has a multiple root near } x\}. \end{cases}$$

4.1 The Shub-Smale approach

In Shub and Smale (1992), the two authors are interested in defining, in the general framework of systems of polynomial equations, a distance to singularity, (or a distance to the discriminant variety) in such a way that a generalized form of Theorem 2.1 remains valid.
This is essentially achieved by considering the constrained distance Δ (which yields $\Delta = 1/K$). But Shub and Smale (1992) contains no indication that Δ may not be the minimal distance.

4.2 The Demmel approach

Demmel is primarily concerned with δ, although he also discusses particular results for Δ (Demmel (1987, Theorem 3 p. 260 and Theorem 10 p. 271)). He establishes for δ the asymptotic upper and lower bounds (valid as $K \longrightarrow \infty$):

$$\frac{a}{K^2} \leq \delta \leq \frac{b}{K}, \tag{2}$$

where a and b are constants. Although Demmel does consider δ and Δ, he does not call the attention of the reader to such a distinction. On the contrary, the many comments in Demmel (1987, 1990) reflect the opinion that in most cases δ approximatively behaves like $1/K$ or, in other words, that $1/K$ gives a reliable estimate of the minimal distance δ. The two given examples clearly illustrate that this need not be the case.

4.3 Our point of view

Is it essential to distinguish between the constrained and minimal distances to singularity? We believe that the answer is yes for the following reasons:

- To be able to extend Theorem 2.1 straightforwardly, the price to pay is to consider Δ where only F is allowed to vary, but x remains fixed. As a result such a constrained distance may be much larger than the minimal one. Therefore, it is misleading to call Δ the "distance to singularity", unless one takes into account the possibility that in reality $\Delta \gg \delta$, so that $1/K$ may not estimate δ reliably; the singularity may be much closer than indicated by $1/K$.

- In finite precision computations, an essential parameter is what we call the "distance to singularity viewed by the computer" (see Chatelin and Frayssé (1993, Chap. 5, par. 5.2)), that is the maximal size of perturbation to which a regular problem can be subjected while remaining regular for the computer. Such a distance is in practice often a good approximation of δ. This reflects the fact that the actual computation at a regular point x is influenced by the presence of the closest singularity y in the neighbourhood of x. That is why we find results such as (2) which relates δ to K, to be of *much more computational significance* than the equality $\Delta = 1/K$.

5 A conjecture about δ

Our computer experiments on multiple eigenvalues and roots of polynomials lead us to propose the following conjecture to refine (2):

Conjecture 5.1 *If x is close to a Hölder-singularity of order $\gamma < 1$, then*

$$\delta = \frac{c}{K^{\frac{1}{1-\gamma}}}, \tag{3}$$

where c is a constant.

For $0 < \gamma \leq 1/2$, the upper bound in (2) corresponds to the limit $\gamma \longrightarrow 0$, and the lower bound corresponds to $\gamma = 1/2$. For roots of multiplicity m, $\gamma = 1/m$, hence $2 \leq m < \infty$. Therefore, the conjecture is, of course, in agreement with (2), but is much more precise.

Another reason that (3) is more appealing than $\Delta = 1/K$ from a computational point of view is the fact that (3) contains the order γ in the exponent $1/(1-\gamma)$. Indeed, γ is the order of the nearby singularity, an information about the computation that is not disclosed by the equality $\Delta = 1/K$.

6 Checking the conjecture on the computer

Conjecture 5.1 has to be confronted with the reality of computations. This can be done by using the computer to test the effect of instability by working on samples of randomly perturbed problems. From a statistical analysis of the computed samples, one can retrieve essential characteristics of the singularities, as they are seen by the computer. All the necessary statistical tools form the basis of the methodology called PRECISE (**PR**ecision **E**stimation and **C**ontrol **I**n **S**cientific and **E**ngineering computing), proposed in 1988 by Chatelin (1988a, 1989). This approach permits one to estimate the condition number K of the problem and its distance to singularity δ. This is achieved by a careful statistical analysis of the effect, on the computed solution, of random perturbations on **the data**, the random perturbations being taken from a specified class of perturbations. Of course, the algorithm used to solve $F(x) = 0$ should be backward stable. The relative perturbation size t varies from machine precision to 1. For each t, the method PRECISE computes an indicator K_t wich gives information on the stability of the mathematical problem. Roughly speaking, K_t compares the perturbations on the data $\|\Delta y\|$ and those on the solution $\|\Delta x\|$.

The generic behaviour for the indicator K_t is given in Figure 1. The x-axis is the perturbation size t. The graph has a logarithmic scale on both axes. When $t \leq t_0$, the estimate K_t appears constant (in fact, it grows very slowly). When t tends to machine precision, the indicator K_t gives an estimation $K_\sharp$ of the asymptotic condition number K, provided K is not too large with respect to the current machine precision. When $t \geq t_0$, K_t decreases. The perturbation size t_0 for which the behaviour of $t \longmapsto K_t$ changes, that is, ceases to be constant, is called the **dangerous border**. For a perturbation of amplitude $t > t_0$, the **computational process** looks **singular** to the computer. In other words, if one uses a computer with a precision $\Psi \geq t_0$, then the computation of the solution is not reliable. The value t_0 measures the maximum perturbation a problem can bear while keeping a given level of regularity. It has been checked (Frayssé (1992)) that t_0 is a good estimate of the distance to singularity δ. If K_t is not infinite for $t = t_0$, this is because a perturbation achieving the singularity is never realized in practice via random perturbations. This point is analysed in more detail in Chatelin and Frayssé (1993). At $t = t_0$, the regularity of the process, as seen by the computer, changes so that when $t \geq t_0$, K_t decreases according to the new (and weaker) degree of regularity. Our experience is that K_t varies like $t^{\gamma-1}$ (which appears as a straight line of slope $\gamma - 1$ on the plot). We give an example of this in the next section.

7 Transition from a simple to a multiple defective eigenvalue

Define the matrix $M(a,b)$ by

$$M(a,b) = \begin{pmatrix} -1-a & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1+b \end{pmatrix},$$

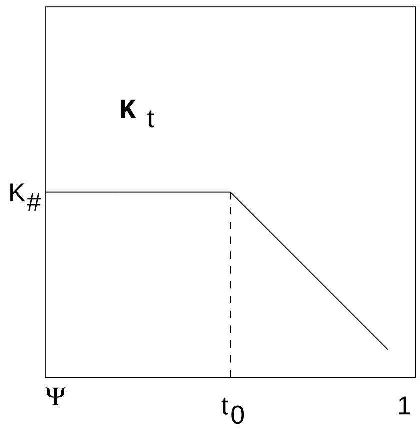

Figure 1: *Statistical estimates of the linear condition number in a log-log scale*

and $A(a,b) = QM(a,b)Q^T$, where Q is an orthonormal matrix is provided by the MATLAB routine *orthog* taken from the collection of test matrices in Higham (1991). We are interested in two cases:

1. $b = -1$: the spectrum of $A(a,-1)$ is $\Lambda = \{-1-a, -1, -2\}$. As a approaches 0, the eigenvalue -1 tends to become a defective eigenvalue of algebraic multiplicity $m = 2$ and of ascent $l = 2$.

2. $b = a$: the spectrum of $A(a,a)$ is $\Lambda = \{-1-a, -1, -1+a\}$. As a approaches 0, the eigenvalue -1 tends to become a defective eigenvalue of algebraic multiplicity $m = 3$ and of ascent $l = 3$.

The eigenvalues are computed by means of the algorithm QR which is backward stable. All the experiments have been performed on a SUN SPARC 10 workstation using MATLAB 4. Machine precision is $\Psi = 2^{-52} \sim 10^{-16}$. We report here the experiments done using normwise perturbations. All the graphs are drawn using a logarithmic scale on both axes. The x-axis shows the size t of the perturbation and the y-axis shows the values of the statistical indicator K_t.

Figure 2 shows the mapping $t \longmapsto K_t$ obtained for the four matrices $A(10^{-4}, -1)$, $A(10^{-7}, -1)$, $A(10^{-3}, 10^{-3})$ and $A(10^{-5}, 10^{-5})$. On the two upper (resp. lower) subplots, the theoretical map $t \longmapsto t^{(1-l)/l}$ for $l = 2$ (resp. $l = 3$) is shown by a continuous (resp. dashed) line. Depending on the choice of the parameters a and b, we observe on the plots a **dangerous** border $t_0(a,b)$, whose values are given in Table 1, for 7 choices of a, and 2 choices of b.

When $a = 10^{-4}$ and $b = -1$, the map representing K_t presents two areas:

- area 1: for $\Psi \le t \le t_0(a,-1)$, K_t appears constant.

a	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
$t_0(a,-1)$	10^{-3}	10^{-5}	10^{-7}	10^{-9}	10^{-11}	10^{-13}	$\leq \Psi$
$t_0(a,a)$	10^{-4}	10^{-7}	10^{-10}	10^{-13}	$\leq \Psi$	$\leq \Psi$	$\leq \Psi$

Table 1: *Dangerous borders $t_0(a,-1)$ and $t_0(a,a)$*

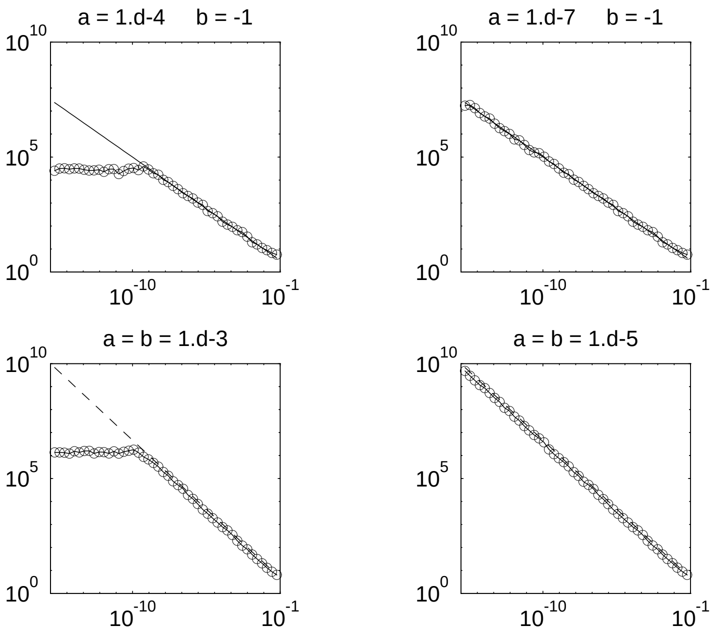

Figure 2: *Behaviour of K_t for various values of a and b*

- area 2: for $t \geq t_0(a, -1)$, K_t decreases and is parallel to $t \longmapsto t^{(1-2)/2} = t^{-1/2}$.

These two areas can be analysed in the following way:

- for $\Psi \leq t \leq t_0(a, -1)$, the ascent of the eigenvalue -1 is $l = 1$; -1 is simple and the regularity of the problem is 1.
- for $t \leq t_0(a, -1)$, $-1 - a$ is viewed by the computer as part of a Jordan block of size 2 associated with -1; -1 becomes double defective with an ascent $l = 2$. The regularity of the problem is now $1/2$.

We can say that the computer "sees" the problem as the computation

- of a simple eigenvalue in area 1,
- of a defective eigenvalue of ascent $l = 2$, in area 2.

The subplot associated with $a = b = 10^{-3}$ now shows the transition from a simple eigenvalue to a triple defective eigenvalue. The transition is the same as the one described above, except that in area 2, K_t now varies as $t \longmapsto t^{(1-3)/3} = t^{-2/3}$. In the case $(a, b) = (10^{-7}, -1)$ (resp. $(a, b) = (10^{-5}, 10^{-5})$), one sees no dangerous border. The dangerous border $t_0(a, b)$ which occurs in the case $(a, b) = (10^{-4}, -1)$ (resp. $(a, b) = (10^{-3}, 10^{-3})$), would also take place for the case $(a, b) = (10^{-7}, -1)$ (resp. $(a, b) = (10^{-7}, -1)$, but for a perturbation size less than Ψ. In fact, it is not visible because the current machine precision ($\Psi \sim 10^{-16}$) is not sufficient. For a computer providing a high enough accuracy, such a dangerous border could become visible because there would possibly exist a range of perturbations for which the eigenvalue $-1 - a$ (resp. $-1 - a$ and $-1 + a$) would appear as simple.

In both cases, we observe that the change of regularity occurs for a distance to singularity which is proportional to the reciprocal of the *square* ($b = -1$) or of *the power* $3/2$ ($b = a$) of the condition number. Indeed one has

- for $(a, b) = (10^{-4}, -1)$: $t_0(a, b) = 10^{-9}$ and $K_\sharp = 3\ 10^4$. Then $t_0(a, b) \sim 1/K_\sharp^2$.
- for $(a, b) = (10^{-3}, 10^{-3})$: $t_0(a, b) = 10^{-10}$ and $K_\sharp = 2\ 10^6$. Then $t_0(a, b) \sim 1/K_\sharp^{\frac{3}{2}}$.

These two examples illustrate very clearly the conjecture presented in Section 5. Indeed, we found here that the distance to singularity t_0 seen by the computer satisfies the law

$$t_0 \propto \frac{1}{K_\sharp^{\frac{l}{l-1}}},$$

where l is the ascent of the eigenvalue. Therefore, this confirms the fact that the degree of regularity γ ($\gamma = 1/l$ here) plays a role in the distance to singularity as seen by the computer.

8 Conclusion

We have shown that there are several ways to extend the Turing theorem ($\delta = 1/K$) to nonlinear problems. The extension $\Delta = 1/K$ is valid if one considers a constrained distance to singularity Δ which might be larger than the minimal distance δ to singularity. For this minimal distance, we conjecture that $\delta = c/K^{\frac{1}{1-\gamma}}$. This formula admits as special cases the upper and lower bounds presented by Demmel (1987). In our opinion, the interesting feature of the conjecture is that it involves the order γ of the singularity.

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