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ILL-CONDITIONEDNESS NEEDS NOT BE COMPONENTWISE NEAR TO ILL-POSEDNESS FOR LEAST SQUARES PROBLEMS

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Abstract. The condition number of a problem measures the sensitivity of the answer to small changes in the input, where "small" refers to some distance measure. A problem is called ill-conditioned if the condition number is large, and it is called ill-posed if the condition number is infinity. It is known that for many problems the (normwise) distance to the nearest ill-posed problem is proportional to the reciprocal of the condition number. Recently it has been shown that for linear systems and matrix inversion this is also true for componentwise distances. In this note we show that this is no longer true for least squares problems and other problems involving rectangular matrices. Problems are identified which are arbitrarily ill-conditioned (in a componentwise sense) whereas any componentwise relative perturbation less than 1 cannot produce an ill-posed problem. Bounds are given using additional information on the matrix.

Key words. Componentwise distance, condition number, ill-posed, least squares, pseudoinverse, underdetermined linear systems
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We first repeat some well known facts about condition numbers for normwise and componentwise perturbations. Consider the matrix

$$A = A(e) := \begin{pmatrix} 1 & e & 0 \\ 0 & 1 & 1 \\ 1 & 0 & e \end{pmatrix} \quad \text{for } 0 \neq e \in \mathbf{R}.$$

For small values of e, a small (normwise) change of the matrix components produces a singular matrix. Indeed, $A+\Delta$ is singular for $\Delta = \begin{pmatrix} 0 & -e & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -e \end{pmatrix}$, and $||\Delta||_2 = ||\Delta||_\infty = ||\Delta||_1 = e$. However, the matrix Δ represents a large *componentwise relative* perturbation of the entries A_{12} and A_{33}, and expanding the determinant of A by Cramer's rule it is clear that *any* componentwise relative perturbation of A less than 1 cannot produce a singular matrix.

The problem of matrix inversion of A is ill-conditioned in a normwise sense because small normwise perturbations of A may produce large normwise changes of A^{-1}. Likewise, the problem of matrix inversion of A is *well-conditioned* subject to componentwise relative perturbations of A. This is because a small componentwise relative perturbation of A causes a small relative change of the determinant of A (as the sum of two numbers of the same sign), and the determinant of all 2×2 submatrices of A is equal to the product of two (sub)matrix entries.

What is true in this specific example turned out to be a general fact: If the problem of matrix inversion is ill-conditioned, then the distance to the nearest singular matrix is small using the same distance measure, no matter whether normwise or componentwise distances are used. In this note we will investigate whether this can be extended to other problems.

Consider for a real $m \times n$ matrix A and a real vector b with m components the following five problems (a pseudoinverse always refers to the Moore-Penrose or (1,2,3,4)

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inverse):

i) A system of linear equations $Ax = b$ for $m = n$,
ii) matrix inversion A^{-1} for $m = n$,
iii) computation of the pseudoinverse A^+ for $m \neq n$,
iv) a least squares problem $||Ax - b||_2 = \text{Min!}$ for $m > n$,
v) an underdetermined linear system $||x||_2 = \text{Min!}$ subject to $||Ax - b||_2 = \text{Min!}$ for $m < n$.

For a small perturbation of the data the change in the solution of one of these problems can be estimated by means of the condition number. Define for a nonsingular square matrix A,

$$\kappa(A) := ||A^{-1}|| \cdot ||A|| \, . \tag{1}$$

For simplicity we use throughout this note the spectral norm. We mention that most of the following results are valid for other norms as well.

Consider a perturbation $\tilde{A}$ of A with $||\tilde{A} - A|| \le \varepsilon \cdot ||A||$. If, for any right hand side, $\tilde{x}$ is the solution of the perturbed system $\tilde{A}\tilde{x} = b$, then [11, Theorem III.2.11]

$$\frac{||\tilde{x} - x||}{||\tilde{x}||} \le \varepsilon \cdot \kappa(A) \, , \tag{2}$$

and for nonsingular $\tilde{A}$ [11, Corollary III.2.7]

$$\frac{||\tilde{A}^{-1} - A^{-1}||}{||\tilde{A}^{-1}||} \le \varepsilon \cdot \kappa(A) \, . \tag{3}$$

When replacing $\tilde{x}$, $\tilde{A}^{-1}$ by the true solution x, A^{-1} in the denominator of (2), (3), respectively, the right hand sides is to be replaced by $\varepsilon \cdot \kappa(A)/(1 - \varepsilon \cdot \kappa(A))$. Moreover, these bounds are attainable up to a small factor (see [5, Theorem 7.2], [11, Corollary III.2.7] and the discussion over there). This gave reason to call $\kappa(A)$ the *condition number of the matrix* (rather than of a problem).

The bounds (2) and (3) look very similar for the other three problems involving rectangular matrices. The definition of the condition number (1) is generalized to a rectangular matrix of full rank into

$$\kappa(A) := ||A^+|| \cdot ||A|| \, . \tag{4}$$

Then, for a perturbed matrix $\tilde{A}$ with $||\tilde{A} - A|| \le \varepsilon \cdot ||A||$ and $\text{rank}(\tilde{A}) = \text{rank}(A)$, it is [11, Corollary III.3.10]

$$\frac{||\tilde{A}^+ - A^+||}{||\tilde{A}^+||} \le \varepsilon \cdot \sqrt{2} \cdot \kappa(A) \, .$$

Similarly, for $\varepsilon \cdot \kappa(A) < 1$ and any right hand side, the solution x of the original problem and the solution $\tilde{x}$ of the perturbed problem with $r = Ax - b$, $\tilde{r} = \tilde{A}\tilde{x} - b$, satisfy [4, Theorem 5.3.1]

$$\frac{||\tilde{r} - r||}{||b||} \le \varepsilon \cdot (1 + 2 \cdot \kappa(A)) + \mathcal{O}(\varepsilon^2)$$

for least squares problems, and [4, Theorem 5.7.1]

$$\frac{||\tilde{x} - x||}{||x||} \le \varepsilon \cdot 2 \cdot \kappa(A) + \mathcal{O}(\varepsilon^2)$$

for underdetermined linear systems. Therefore $\kappa(A) := ||A^+|| \cdot ||A||$ is often called the condition number of a (full-rank) rectangular matrix. Note that the sensitivity of the solution (rather than of the residual) of least squares problems is the square of $\kappa(A)$ [4, Theorem 5.3.1].

It is well known that any of the above five problems becomes ill-posed [12] if and only if the matrix is rank-deficient. The 2-norm distance of a full-rank matrix to the nearest singular matrix is the smallest singular value of A [4, Theorem 2.5.2], which is $||A^+||^{-1}$. Therefore, for full-rank square and rectangular matrices,

$$\min\left\{0 < \varepsilon \in \mathbf{R} \;\middle|\; \exists \tilde{A} \,:\, ||\tilde{A} - A|| \le \varepsilon \cdot ||A||,\ \tilde{A} \text{ rank-deficient}\right\} = \kappa(A)^{-1} \,. \tag{5}$$

This confirms the well known fact that

(6) *the normwise distance to the nearest ill-posed problem of a problem i) to v) is proportional to the reciprocal of $\kappa(A)$.*

This has been shown to be true for a number of other problems in numerical analysis in the classical paper [2].

It seems natural to ask whether this statement is still true for other measures of distance, for example componentwise distances. For this purpose we need an appropriate condition number. We restrict our attention to the practically important case of componentwise relative perturbations but mention that most of the following is valid in a much more general setting, i.e. for componentwise perturbations subject to an arbitrary nonnegative weight matrix [8, **?**].

For a given matrix A (square or rectangular) consider a perturbation $\tilde{A}$ with

$$|\tilde{A} - A| \le \varepsilon \cdot |A|. \tag{7}$$

Here and in the following, absolute value and comparison are always to be understood componentwise. So (7) is equivalent to $|\tilde{A}_{ij} - A_{ij}| \le \varepsilon \cdot |A_{ij}|$ for all i, j. Define for a full-rank matrix A,

$$\operatorname{cond}(A) := ||\, |A^+| \cdot |A|\, || \,. \tag{8}$$

For square matrices this is the so-called Bauer-Skeel condition number. Let $\tilde{A}$ be a perturbation of A satisfying (7). Then for a square matrix A and any right hand side b with $Ax = b$ and $\tilde{A}\tilde{x} = b$ and $\varepsilon \cdot \operatorname{cond}(A) < 1$, it is [11, Corollary III.2.15]

$$\frac{||\tilde{x} - x||}{||x||} \le \varepsilon \cdot \frac{\operatorname{cond}(A)}{1 - \varepsilon \cdot \operatorname{cond}(A)} \,.$$

For a square or underdetermined linear system with full-rank matrix A and $\varepsilon \cdot \operatorname{cond}(A) < 1$, it is [5, (20.8)]

$$\frac{||\tilde{x} - x||}{||x||} \le \varepsilon \cdot 3 \cdot \operatorname{cond}(A) + \mathcal{O}(\varepsilon^2) \,.$$

There are similar, although more involved, estimates for the sensitivity of matrix inversion and least squares problems subject to componentwise relative perturbations (see, for example, [5, Theorem 7.4 and Theorem 19.2]). These estimations contain again $\mathrm{cond}(A)$. Therefore, $\mathrm{cond}(A) := \| \, |A^+| \cdot |A| \, \|$ is sometimes called the *componentwise condition number* of a matrix.

The question is whether some relation similar to (5) can be established in the case of componentwise distances. Define for a full-rank rectangular matrix A,

$$\sigma(A, |A|) := \min \left\{ 0 < \alpha \in \mathbf{R} \;\middle|\; \exists \tilde{A} \, : \, |\tilde{A} - A| \le \alpha \cdot |A|, \; \tilde{A} \text{ rank-deficient} \right\} \; . \tag{9}$$

Definition (9) can be generalized to other nonnegative weight matrices E by replacing $|A|$ by E. In the following, we restrict our attention to the important case of entrywise relative perturbations: $E = |A|$.

Obviously $0 < \sigma(A, |A|) \le 1$. Unlike in the normwise case, a characterization cannot be a simple equality as in (5). This is because Poljak and Rohn showed that computation of $\sigma(A, |A|)$ for square A is NP-hard [7]. Moreover, the definition of $\mathrm{cond}(A)$ still depends on a norm, and improper scaling may produce artificial ill-conditioning [11, p.122f].

Let us first consider the square case, i.e. problems *i)* and *ii)*. In this case we may ask for the optimal scaling, that is for the minimum achievable condition number $\mathrm{cond}(AD)$ for nonsingular diagonal D (the condition number $\mathrm{cond}(A)$ is independent of row scaling for $m \le n$). For ρ denoting the spectral radius it is ([3, §5], see also [1])

$$\inf_D \mathrm{cond}(AD) = \rho(|A^{-1}| \, |A|) \; , \tag{10}$$

where for irreducible $|A^{-1}||A|$ the minimizing diagonal matrix can be computed explicitly from the left and right Perron vector of $|A^{-1}| \cdot |A|$. The question is whether, similar to the normwise case (5), the minimum achievable componentwise condition number is related to the componentwise distance to the nearest rank-deficient matrix. Indeed, it has been shown in [**?**, 8] that for square nonsingular A

$$\frac{1}{\inf_D \mathrm{cond}(AD)} \le \sigma(A, |A|) \le \frac{(3 + 2\sqrt{2})n}{\inf_D \mathrm{cond}(AD)} \; . \tag{11}$$

The left bound has been known for long and is an immediate consequence of Perron-Frobenius theory: If $A + \Delta = A(I + A^{-1}\Delta)$ is singular for $|\Delta| \le \beta \cdot |A|$ and $\beta := \sigma(A, |A|)$, then $1 \le \rho(A^{-1}\Delta) \le \rho(|A^{-1}\Delta|) \le \rho(|A^{-1}||\Delta|) \le \beta \cdot \rho(|A^{-1}||A|)$. The right bound of (11) is the difficult part; a consolidated proof of this inequality will appear in SIAM Review [10]. The right bound is sharp up to the factor $3 + 2\sqrt{2}$ for any n [**?**]. In words:

(12) *The componentwise distance to the nearest rank-deficient matrix is proportional to the reciprocal of the minimum achievable componentwise condition number for square matrices.*

That means, if a linear system or the problem of matrix inversion is ill-conditioned subject to componentwise relative perturbations of the matrix, then a small componentwise relative perturbation produces an ill-posed problem.

It seems natural to ask whether this statement is still true for problems *iii)* to *v)*. First, we face the same problem as in the square case that $\mathrm{cond}(A)$ depends on a norm. For full-rank least squares problems it is

$$\inf_D \mathrm{cond}(AD) = \rho(|A^+| \cdot |A|) \quad \text{for } A \in M_{mn}(\mathbf{R}), \; m \ge n \; . \tag{13}$$

This is because $(AD)^+ = D^{-1}A^+$, and setting $B := |A^+| \cdot |A|$, (13) is equivalent to

$$\inf_D ||D^{-1}BD|| = \rho(B) \quad \text{for } B \in M_n(\mathbf{R}),\ B \geq 0,$$

which can be shown along the lines of the proof of Theorem 5.2 in [3]. Unlike the corresponding condition number for square matrices, $\kappa(A)$ is not independent of diagonal row scaling. However, it does not make sense to use an infimum of $\kappa(DA)$ over diagonal D, because this changes the problem, and putting zeros in appropriate diagonal positions of D readily produces the (usual) condition number of some square matrix out of A. Furthermore, for a least squares problem row scaling is usually related to uncertainties in the right hand side (cf. [6]). The same remarks apply similarly to undetermined linear systems.

In any case, for square as well as for rectangular matrices, it is

$$(14)\ \rho(|A^+| \cdot |A|) \leq \text{cond}(A) \quad \text{and} \quad \rho(|A^+|\,|A|) \leq ||A^+||_\infty ||A||_\infty \leq \sqrt{mn} \cdot \kappa(A)\ .$$

If a statement in the spirit of (12) would be true for one of the problems *iii)* to *v)*, then for a rectangular matrix A with $\rho(|A^+| \cdot |A|)$ being large, and henceforth $\text{cond}(A)$ being large, a small componentwise relative perturbation must produce a rank-deficient matrix. In the following we show that this is not true in general.

Suppose A is a real $m \times n$ matrix of full rank $k = \min(m, n)$, and $\tilde{A}$ is some rank-deficient perturbation of A. The rank-deficiency of $\tilde{A}$ is equivalent to the fact that all $k \times k$ submatrices of $\tilde{A}$ are singular. Therefore, definition (9) yields for a real $m \times n$ matrix A of full rank $k = \min(m, n)$

$$(15) \qquad \max_{A^*} \sigma(A^*, |A^*|) \geq \sigma(A, |A|) \geq \min_{A*} \sigma(A^*, |A^*|)\ ,$$

where the maximum and minimum is taken over all $k \times k$ submatrices A^* of A. Consider the following matrix

$$(16) \qquad A = A(\varepsilon) := \begin{pmatrix} 0 & -1 & 0 \\ -1 & 1 & 1 \\ 0 & 1 & \varepsilon \\ -1 & -1 & 1 \end{pmatrix} \quad \text{for } 0 \neq \varepsilon \in \mathbf{R}\ .$$

Then $\det(A^TA) = 6\varepsilon^2$ and A is of full rank. Furthermore, for $|\varepsilon| < 2/3$,

$$|A^+| \cdot |A| = \frac{1}{3|\varepsilon|} \begin{pmatrix} 2 & 6 & 2+3|\varepsilon| \\ 2|\varepsilon| & 3|\varepsilon| & 2|\varepsilon| \\ 2 & 6 & 2+3|\varepsilon| \end{pmatrix}$$

implies $\rho(|A^+| \cdot |A|) > \varepsilon^{-1}$. By (14), $\kappa(A)$ is large for small ε, and by (6) a small *normwise* perturbation must produce a rank-deficient matrix. Indeed, changing A_{33} into 0 yields a rank-2 matrix.

All three problems *iii)* to *v)* are also ill-conditioned subject to small relative perturbations of A. It is (the numbers were computed using Maple [13])

$$A^+ = \frac{1}{6\varepsilon} \cdot \begin{pmatrix} 2 & -2-3\varepsilon & 6 & 2-3\varepsilon \\ -2\varepsilon & 2\varepsilon & 0 & -2\varepsilon \\ 2 & -2 & 6 & 2 \end{pmatrix},$$

whereas perturbing A into $\tilde{A}$ by changing the (4,3)-component into $1-\delta$ yields

$$(\tilde{A}^+)_{11} = \frac{1}{6\varepsilon} \cdot \left(2 + \left(\frac{10}{3\varepsilon} - 1 \right) \cdot \delta + \mathcal{O}(\delta^2) \right) \; .$$

Therefore, the sensitivity of $(\tilde{A}^+)_{11}$ with respect to a componentwise relative perturbation of A_{43} is larger than ε^{-1}. Thus the problem of computing the pseudoinverse of A, the least squares problem with right hand side $(1,0,0)^T$, and the underdetermined linear system with right hand side $(1,0,0,0)^T$ is indeed ill-conditioned for componentwise relative perturbations.

On the other hand, we know from (15) that the componentwise distance to the nearest rank-deficient matrix is bounded below by the componentwise distance of the upper 3×3 matrix of A to the nearest singular matrix. The determinant of this matrix is $-A_{12}A_{21}A_{33}$, and any componentwise relative perturbation less than 1 of A cannot produce a singular matrix. Summarizing:

If the problem of
computing the pseudoinverse,
a least squares problem,
or an underdetermined linear system
is ill-conditioned subject to componentwise relative perturbations of the matrix entries, then the problem need not *be near an ill-posed problem subject to componentwise relative perturbations.*

In fact, in our example the componentwise distance to the nearest rank-deficient matrix is equal to the distance to the rank-0 matrix. From the 4×3 example (16) it is easy to derive examples of larger dimensions.

The main difference between the square and the rectangular case is that, for $k = \min(m,n)$, in the latter case a perturbation has to lower the rank of *every* $k \times k$ submatrix simultaneously, whereas in the first case only *one* matrix, the given matrix, must become singular. Another explanation uses that for $\tilde{A} := A + \Delta$ the matrix $\tilde{A}^T\tilde{A} = (A+\Delta)^T(A+\Delta)$ must become singular for a perturbation Δ. For a similar reason, a symmetric matrix, the inversion of which is sensitive with respect to *symmetric* componentwise relative perturbations, need not be near a singular matrix with respect to symmetric componentwise relative perturbations [9].

For the square cases *i*) and *ii*) we have with (11) general two-sided bounds for the ratio between the componentwise distance to the nearest ill-posed problem and the reciprocal of the condition number. Example (16) shows that this ratio is, in general, unbounded for the problems *iii*) to *v*). The question remains whether bounds are possible using additional information on A. We are interested in bounds for the quantity

$$\gamma := \sigma(A, |A|) \cdot \mathrm{cond}(A) = \sigma(A, |A|) \cdot \| \, |A^+| \cdot |A| \, \|$$

for full-rank rectangular $A \in M_{mn}(\mathbf{R})$. Note that, unlike (11), we use the actual condition number, not an optimal condition number subject to some scaling. Such bounds are indeed possible.

A general *lower* bound without further assumptions on A can be established similar to the square case. Let full-rank $A \in M_{mn}(\mathbf{R})$, $m \geq n$, and rank deficient

$A+\Delta=(I+\Delta A^+)A$ with $|\Delta| \le \sigma(A,|A|)\cdot|A|$ be given. Then $I+\Delta A^+$ is rank-deficient and

$$(17) \qquad 1 \le \rho(\Delta A^+) = \rho(A^+\Delta) \le \rho(|A^+|\,|\Delta|) \le \sigma(A,|A|)\cdot\rho(|A^+|\cdot|A|) = \gamma.$$

For $m<n$ the same argument using $A+\Delta = A(I+A^+\Delta)$ applies.

For an upper bound we need additional information on A. Denote

$$\mu := \min_{i,j} |A|_{ij} \quad \text{and} \quad M := \max_{i,j} |A|_{ij}.$$

For the singular value decomposition $A=\sum \sigma_i u_i v_i^T$ with smallest singular value σ_k, $k=\min(m,n)$, the matrix $A-\sigma_k u_k v_k^T$ is rank-deficient. For $(1)_{mn}$ denoting the $m\times n$ matrix of all 1's,

$$|\sigma_k u_k v_k^T| \le \sigma_k\cdot(1)_{mn} \le \mu^{-1}\sigma_k\cdot|A| = \mu^{-1}||A^+||^{-1}|A|\,.$$

Hence $\sigma(A,|A|) \le \{\mu\cdot||A^+||\}^{-1}$. On the other hand [5, Table 6.2],

$$\begin{aligned} \mathrm{cond}(A) = ||\;|A^+|\cdot|A|\;|| &\le \sqrt{||\;|A^+|\cdot|A|\;||_1\;||\;|A^+|\cdot|A|\;||_\infty} \\ &\le \sqrt{||A^+||_1\;||A||_1\;||A^+||_\infty\;||A||_\infty} \\ &\le M\sqrt{mn}\;\sqrt{||A^+||_1\;||A^+||_\infty} \\ &\le M(mn)^{3/4}\;||A^+||\,. \end{aligned}$$

Together with (17) and (16) this proves the following result for square and for rectangular matrices. For square matrices a weaker result of this kind is [3, Theorem 5.4].

THEOREM 1.1. *Suppose* $A\in M_{mn}(\mathbf{R})$ *has full rank, suppose* $A_{ij}\ne 0$ *for all* i,j *, and define*

$$\varphi := \frac{\max\ |A_{ij}|}{\min\ |A_{ij}|}.$$

Then

$$\frac{1}{\mathrm{cond}(A)} \le \sigma(A,|A|) \;\le\; \frac{\varphi\cdot(mn)^{3/4}}{\mathrm{cond}(A)}\,,$$

where the componentwise condition number $\mathrm{cond}(A)$ *is defined by* (8)*, and the componentwise distance* $\sigma(A,|A|)$ *to the nearest rank-deficient problem subject to relative componentwise perturbations is defined by* (9).

Without the assumption $A_{ij}\ne 0$*, the product* $\sigma(A,|A|)\cdot\mathrm{cond}(A)$ *can be arbitrarily large for* $m\ne n$*,* $m\ge 4$*,* $n\ge 3$.

The result can be interpreted as follows. The closer the entries of A are in magnitude, that means the more a componentwise *relative* perturbation becomes a componentwise *absolute* perturbation, the closer are the componentwise distance to the nearest rank-deficient matrix and the reciprocal of the condition number.

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