SPECTRAL CONDITION NUMBERS OF ORTHOGONAL PROJECTIONS AND FULL RANK LINEAR LEAST SQUARES RESIDUALS*

JOSEPH F. GRCAR[†]

Abstract. A simple formula is proved to be a tight estimate for the condition number of the full rank linear least squares residual with respect to the matrix of least squares coefficients and scaled 2-norms. The tight estimate reveals that the condition number depends on three quantities, two of which can cause ill-conditioning. The numerical linear algebra literature presents several estimates of various instances of these condition numbers. All the prior values exceed the formula introduced here, sometimes by large factors.

Key words. residual, projection, linear least squares, condition number, applications of functional analysis

AMS subject classifications. 65F35, 62J05, 15A60

1. Introduction.

1.1. Purpose. Least squares residuals are quite important numerically. The residuals measure the quality of fits in regression analysis, and forming orthogonal projections is an essential step in many iterative algorithms for linear equations or matrix eigenvalues.

This paper determines a tight estimate for the condition number of the residual in full rank least squares problems. Equivalently, the condition number of orthogonal projections into the span of linearly independent vectors is also estimated. The condition numbers are with respect to the matrix of least squares coefficients and with respect to scaled 2-norms. The condition number of the residual, like the solution, is the value of an optimization problem that does not have an explicit formula but which does have a tight estimate.

This introduction provides some background material. Section 2 discusses the evaluation of condition numbers from Jacobian matrices. Section 3 describes the tight estimate of the condition number and provides an example; this material is appropriate for classroom presentation. Section 4 proves that the condition number varies from the estimate within a factor of $\sqrt{2}$; the linear algebra is complicated but straightforward given an identity from a previous paper (Grcar, 2009). Section 5 compares the results to the literature. Section 6 discusses the application to projections and to iterative algorithms.

1.2. Prior Work. Conditioning with respect to perturbations of the matrix A is the most interesting aspect of least squares problems,

$$x = \arg\min \|b - Au\|_2$$
 $r = b - Ax$. (1.1)

The condition numbers $\chi_x(A)$, of x with respect to A for various norms, have been studied in dozens of papers and books since Golub and Wilkinson (1966) discovered the condition number for 2-norms can depend on the square of the matrix condition number. Thus, it was equally surprising when Björck (1967, p. 16, eqn. 7.7) discovered the conditioning of the residual is independent of the square.¹ Even so, Björck's original formula turned out to be an overestimate. Roughly the same formula is still found in many textbooks (section 5.3).

Wedin (1973, p. 224, eqn. 5.4) derived a perturbation bound for the residual with respect to A again for 2-norms. This paper shows that Wedin's bound contains an estimate for $\chi_r(A)$ that is accurate within a factor of 2. Wedin noted that his perturbation bound could be "almost

^{*}PLEASE READ AND CITE THE CORRECTED, PUBLISHED ARTICLE THAT CAN BE ACCESSED THROUGH THE DOI LINK ON THE ARXIV PAGE FOR THIS DOCUMENT.

[†]6059 Castlebrook Drive, Castro Valley, CA 94552 USA (jfgrcar@comcast.net, or na.grcar@na-net.ornl.gov). ¹Björck derived a bound for the sum of condition numbers with respect to A and b, $\chi_r(A) + \chi_r(b)$.

attained" (p. 225). However, (p. 226) he also remarked that his paper only demonstrated near attainment for a perturbation bound on the least squares solution (not the residual). Thus the published literature has no prior proof of attainment for an error bound of the residual.

Geurts (1982) and Gratton (1996) have used Jacobian matrices to derive condition numbers, or estimates of condition numbers, for least squares solutions. Their results and those of Björck (1967), Malyshev (2003), and Wedin (1973) for the condition number of the solution are summarized by Grcar (2009). There has been no similar determination of condition numbers based on Jacobian matrices for the residual. The spectral condition number of the residual, like the solution, is the value of an optimization problem that does not have an explicit formula but which does have a tight estimate. No tight estimates for the condition number of the least squares residual have been established previously.

2. Condition numbers.

2.1. Error bounds and definitions of condition numbers. "Perturbation bounds" are used in numerical analysis to limit the sensitivity of the solution of a problem to changes in the initial data. Such bounds are customarily derived using matrix-vector algebra and norms; the coefficients of the data perturbations in these bounds are sometimes referred to as condition numbers. For example, in one of the earliest books on rounding error analysis, Wilkinson (1963, p. 29) wrote "we shall refer to [the coefficients] as condition numbers" Many numerical analysts probably agree with Wilkinson in the interest of deriving error bounds, but the name "condition number" is used sparingly because the coefficients are only upper limits for condition numbers unless the error bounds are the smallest possible, equivalently, unless the error bounds are attained. Malyshev (2003, p. 1187) observed, "the bounds are commonly accepted as condition numbers, and any discussion about their sharpness is usually avoided."

The oldest way to derive perturbation bounds is by differential calculus. If y = f(x) is a vector valued function of the vector x whose partial derivatives are continuous, then the partial derivatives give the best estimate of the change to y for a given change to x

$$\Delta y = f(x + \Delta x) - f(x) \approx J_f(x) \,\Delta x \tag{2.1}$$

where $J_f(x)$ is the Jacobian matrix of the partial derivatives of y with respect to x. The magnitude of the error in the first order approximation (2.1) is bounded by Landau's little $o(||\Delta x||)$ for all sufficiently small $||\Delta x||^2$. Thus $J_f(x) \Delta x$ is the unique linear approximation to Δy in the vicinity of x.³ Taking norms produces a perturbation bound,

$$\|\Delta y\| \le \|J_f(x)\| \|\Delta x\| + o(\|\Delta x\|).$$
(2.2)

Equation (2.2) is the smallest possible bound on $\|\Delta y\|$ in terms of $\|\Delta x\|$ provided the norm for the Jacobian matrix is induced from the norms for Δy and Δx . In this case for each xthere is some Δx , which is nonzero but may be chosen arbitrarily small, so the bound (2.2) is attained to within the higher order term, $o(\|\Delta x\|)$. There may be many other ways to define condition numbers, but because equation (2.2) is the smallest possible bound, any definition of a condition number for use in bounds equivalent to (2.2) must arrive at the same value, $\chi_y(x) = \|J_f(x)\|$.⁴ The matrix norm may be too complicated to have an explicit formula, but tight estimates can be derived as in this paper.

²The $o(||\Delta x||)$ agreement is independent of the norm because all norms for finite dimensional spaces are equivalent (Stewart and Sun, 1990, p. 54, thm. 1.7).

³Any other linear function added to $J_f(x) \Delta x$ differs from Δy by $\mathcal{O}(||\Delta x||)$ and therefore does not provide a $o(||\Delta x||)$ approximation.

⁴A theory of condition numbers in terms of Jacobian matrices was developed by Rice (1966, p. 292, thm. 4). See also Trefethen and Bau (1997, p. 90) for the present definition.

2.2. One or separate condition numbers. Many problems depend on two parameters u, v which may consist of the entries of a matrix and a vector (for example). In principle it is possible to treat the parameters altogether.⁵⁶ A condition number for y with respect to joint changes in u and v requires a common norm for perturbations to both. Such a norm is

$$\max\left\{ \|\Delta u\|, \|\Delta v\| \right\}. \tag{2.3}$$

A single condition number then follows that appears in an optimal error bound,

$$\|\Delta y\| \le \|J_f(u,v)\| \max\{\|\Delta u\|, \|\Delta v\|\} + o\left(\max\{\|\Delta u\|, \|\Delta v\|\}\right).$$
(2.4)

The Jacobian matrix $J_f(u, v)$ contains the partial derivatives of y = f(u, v) with respect to the entries of both u and v. The value of the condition number is again $\chi_y(u, v) = ||J_f(u, v)||$ where the matrix norm is induced from the norm for Δy and the norm in equation (2.3).

Because u and v may enter into the problem in much different ways, it is customary to treat each separately. This approach recognizes that the Jacobian matrix is a block matrix

$$J_f(u,v) = \left[J_{f_1}(u) \ J_{f_2}(v) \right]$$

where the functions $f_1(u) = f(u, v)$ and $f_2(v) = f(u, v)$ have v and u fixed, respectively. The first order differential approximation (2.1) is unchanged but is rewritten with separate terms for u and v,

$$\Delta y \approx J_{f_1}(u)\,\Delta u + J_{f_2}(v)\,\Delta v\,,\tag{2.5}$$

and a perturbation bound is obtained by applying the triangle inequality,

$$\|\Delta y\| \le \|J_{f_1}(u)\Delta u + J_{f_2}(v)\Delta v\| + o\left(\max\left\{\|\Delta u\|, \|\Delta v\|\right\}\right)$$

$$\le \|J_{f_1}(u)\| \|\Delta u\| + \|J_{f_2}(v)\| \|\Delta v\| + o\left(\max\left\{\|\Delta u\|, \|\Delta v\|\right\}\right).$$
(2.6)

The coefficients $\chi_y(u) = ||J_{f_1}(u)||$ and $\chi_y(v) = ||J_{f_2}(v)||$ are the separate condition numbers of y with respect to u and v, respectively.

These two different approaches lead to error bounds (2.4, 2.6) that differ by at most a factor of 2. This fact is a property of induced norms. Consider a $p \times (m + n)$ block matrix

$$y = \left[\begin{array}{cc} A & B \end{array} \right] \left[\begin{array}{c} u \\ v \end{array} \right]$$

and suppose norms are given for \mathbb{R}^p , \mathbb{R}^m and \mathbb{R}^n as spaces of column vectors. A norm can be defined for \mathbb{R}^{m+n} as

$$\left\| \begin{bmatrix} u \\ v \end{bmatrix} \right\| = \max\left\{ \|u\|, \|v\| \right\}.$$

These norms for \mathbb{R}^p , \mathbb{R}^m , \mathbb{R}^n , and \mathbb{R}^{m+n} induce norms for A, B, and $[A \ B]$,

$$||A|| = \max_{u \neq 0} \frac{||Au||}{||u||}, \quad ||B|| = \max_{v \neq 0} \frac{||Au||}{||v||}, \quad ||[|A||B|]|| = \max_{u \neq 0 \text{ or } v \neq 0} \frac{||Au| + Bv||}{\max\{||u||, ||v||\}}$$

⁵As will be discussed, Gratton (1996) derived a joint condition number of the least squares solution with respect to a Frobenius norm of the matrix and vector that define the problem.

⁶Gratton (1996) derived a joint condition number of the least squares solution with respect to a Frobenius norm of the matrix and vector that define the problem.

The norm of the block matrix has a simple upper bound,

$$\begin{split} \| \begin{bmatrix} A & B \end{bmatrix} \| &= \max_{u \neq 0 \text{ or } v \neq 0} \frac{\|Au + Bv\|}{\max \{\|u\|, \|v\|\}} \\ &\leq \max_{u \neq 0 \text{ or } v \neq 0} \frac{\|Au\|}{\max \{\|u\|, \|v\|\}} + \max_{u \neq 0 \text{ or } v \neq 0} \frac{\|Bv\|}{\max \{\|u\|, \|v\|\}} \\ &= \max_{u \neq 0} \frac{\|Au\|}{\|u\|} + \max_{v \neq 0} \frac{\|Bv\|}{\|v\|} \\ &= \|A\| + \|B\|, \end{split}$$
(2.7)

and a simple lower bound,

$$||A|| = \max_{u \neq 0} \frac{||Au||}{||u||} = \max_{u \neq 0 \text{ and } v=0} \frac{||Au + Bv||}{\max\{||u||, ||v||\}} \le \max_{u \neq 0 \text{ or } v \neq 0} \frac{||Au + Bv||}{\max\{||u||, ||v||\}} = ||[A \ B]||, \quad (2.8)$$

and similarly $||B|| \leq ||[A \ B]||$. Altogether, from equations (2.7, 2.8),

$$\frac{\|A\| + \|B\|}{2} \le \max\left\{\|A\|, \|B\|\right\} \le \left\|\left[A \ B\right]\right\| \le \|A\| + \|B\|$$
(2.9)

which means that ||A|| + ||B|| overestimates $||[A \ B]||$ by at most a factor of 2. Returning to the Jacobian matrices $A = J_{f_1}(u)$, $B = J_{f_2}(v)$, and $[A \ B] = J_f(u, v)$, equation (2.9) can be rewritten

$$\frac{\chi_y(u) + \chi_y(v)}{2} \le \chi_y(u, v) \le \chi_y(u) + \chi_y(v).$$
(2.10)

Thus, for the purpose of deriving tight estimates of joint condition numbers, it suffices to consider $\chi_y(u)$ and $\chi_y(v)$ separately.

3. Conditioning of the least squares residual.

3.1. Reason for considering full rank problems. For any matrix A and any similarly sized column vector b, the linear least squares problem (1.1) need not have an unique solution x, but it always has an unique residual r = b - Ax = (I - P)b where $P = AA^{\dagger}$ is the orthogonal projection into the column space of A, col(A), and where A^{\dagger} is the pseudoinverse of A. If A has full column rank, then $P = A(A^tA)^{-1}A^t$. Changes to A affect r differently when A does not have full column rank. In that case, $b \in col(A + bz^t)$ for every nonzero right null vector z, so small changes to A can produce large changes to r. In other words, a condition number of r with respect to rank deficient A does not exist or is "infinite." Perturbation bounds in the rank deficient case can be found by restricting changes to the matrix, for which see Björck (1996, p. 30, eqn. 1.4.27) and Stewart and Sun (1990, pp. 136–162). That theory is beyond the scope of the present discussion.

3.2. The condition numbers. This section summarizes the results and presents an example. Proofs are in section 4. It is assumed that A has full column rank and neither the solution x nor the residual r of the least squares problem are zero. The residual is proved to have a condition number $\chi_r(A)$ with respect to A within the limits,

$$\frac{1}{\sqrt{2}} \left| \kappa_2 \sqrt{1 + \left(\frac{\cot(\boldsymbol{\theta})}{\mathbf{v}}\right)^2} \right| \le \chi_r(A) \le \left| \kappa_2 \sqrt{1 + \left(\frac{\cot(\boldsymbol{\theta})}{\mathbf{v}}\right)^2} \right|.$$
(3.1)

The quantities κ_2 , θ , and V are written bold to emphasize they are the only quantities affecting the tight estimate of the condition number; they are defined below. There is also a condition number with respect to *b*,

$$\chi_r(b) = \boxed{\csc(\boldsymbol{\theta})}.$$
(3.2)

These are condition numbers when the following scaled 2-norms are used to measure the perturbations to A, b, and x,

$$\frac{\|\Delta A\|_2}{\|A\|_2}, \qquad \frac{\|\Delta b\|_2}{\|b\|_2}, \qquad \frac{\|\Delta r\|_2}{\|r\|_2}.$$
(3.3)

Like equation (2.6), the two condition numbers appear in error bounds of the form,⁷

$$\frac{\|\Delta r\|_2}{\|r\|_2} \le \chi_r(A) \frac{\|\Delta A\|_2}{\|A\|_2} + \chi_r(b) \frac{\|\Delta b\|_2}{\|b\|_2} + o\left(\max\left\{\frac{\|\Delta A\|_2}{\|A\|_2}, \frac{\|\Delta b\|_2}{\|b\|_2}\right\}\right), \quad (3.4)$$

where $r + \Delta r$ is the residual of the perturbed problem,

$$x + \Delta x = \arg\min_{u} \|(b + \Delta b) - (A + \Delta A)u\|_2.$$
 (3.5)

The quantities in the formulas (3.1, 3.2) are

$$\kappa_{2} = \frac{\|A\|_{2}}{\sigma_{\min}}, \qquad \cot(\theta) = \frac{\|Ax\|_{2}}{\|r\|_{2}} \qquad \mathbf{V} = \frac{\|Ax\|_{2}}{\|x\|_{2}\sigma_{\min}}, \tag{3.6}$$

where κ_2 is the spectral matrix condition number of A (σ_{\min} is the smallest singular value of A), V is van der Sluis's ratio between 1 and κ_2 ,⁸ and θ is the angle between b and col(A).

- 1. κ_2 depends only on the extreme singular values of A.
- 2. θ depends only on the "angle of attack" of b with respect to col(A).
- 3. If A is fixed, then **v** depends on the orientation of b to col(A) but not on θ .⁹

Please refer to Figure 3.1 as needed. If col(A) is fixed, then κ_2 and θ are separate sources of ill-conditioning for the residual. The ratio V can never cause ill-conditioning because it only appears in the denominator of equation (3.1) and V is always at least 1. Indeed, if Ax has comparatively large components in singular vectors corresponding to the largest singular values, then $V \approx \kappa_2$ and V might lessen the ill-conditioning caused by a small θ .

3.3. Conditioning example. This example illustrates the effects of κ_2 , v, and θ on $\chi_r(A)$. It is based on the example of Golub and Van Loan (1996, p. 238). Let

$$A = \begin{bmatrix} 1 & 0 \\ 0 & \alpha \\ 0 & 0 \end{bmatrix}, \quad b = \begin{bmatrix} \beta \cos(\phi) \\ \beta \sin(\phi) \\ 1 \end{bmatrix}, \quad \Delta A = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ -\epsilon & -\epsilon \end{bmatrix},$$

where $0 < \epsilon \ll \alpha, \beta$, and $\alpha < 1$. In this example,

$$x = \begin{bmatrix} \beta \cos(\phi) \\ \frac{\beta}{\alpha} \sin(\phi) \end{bmatrix}, \quad r = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \Delta r = \begin{bmatrix} 1 \\ \frac{1}{\alpha} \\ \beta \cos(\phi) + \frac{\beta}{\alpha} \sin(\phi) \end{bmatrix} \epsilon + \mathcal{O}(\epsilon^2).$$

⁷The constant denominators $||A||_2$ and $||b||_2$ could be discarded from the *o* terms because only the order of magnitude of the terms is pertinent.

⁸Van der Sluis (1975, p. 251) introduced no notation. The Greek letters that look and sound like English v are ν and β , respectively, so it seems best to choose Roman V for van der Sluis.

⁹Because A has full column rank, Ax and x can only vary proportionally when their directions are fixed.



FIG. 3.1. Schematic of the least squares problem, the projection Ax, and the angle θ between Ax and b.

The three terms in the condition number are

$$\kappa_2 = \frac{1}{\alpha}, \qquad \mathbf{V} = \frac{1}{\sqrt{[\alpha \cos(\phi)]^2 + [\sin(\phi)]^2}}, \qquad \cot(\boldsymbol{\theta}) = \beta.$$

These values can be manipulated by choosing α , β and ϕ . The tight upper bound on the condition number with respect to A is

$$\chi_r(A) \le \frac{1}{\alpha} \sqrt{1 + [\alpha\beta\cos(\phi)]^2 + [\beta\sin(\phi)]^2}.$$

The relative change to the residual,

$$\frac{\|\Delta r\|_2}{\|r\|_2} = \frac{1}{\alpha} \sqrt{1 + \alpha^2 + [\alpha\beta\cos(\phi) + \beta\sin(\phi)]^2} \epsilon + \mathcal{O}(\epsilon^2),$$

can made be close to the bound on $\chi_r(A)$ times $\|\Delta A\|_2 / \|A\|_2 = \sqrt{2}\epsilon$. These formulas have been verified using Mathematica (Wolfram, 2003), as have formulas throughout the paper.

4. Derivation of the condition number estimates.

4.1. Choice of Norms. In theoretical numerical analysis especially for least squares problems the 2-norm is preferred because for it the matrix condition number of A^tA is the square of the matrix condition number of A. The norms used in this paper and in many other papers are defined as,

$$\|\operatorname{vec}(\Delta A)\|_{\mathcal{A}} = \frac{\|\Delta A\|_2}{\mathcal{A}}, \qquad \|\Delta b\|_{\mathcal{B}} = \frac{\|\Delta b\|_2}{\mathcal{B}}, \qquad \|\Delta r\|_{\mathcal{R}} = \frac{\|\Delta r\|_2}{\mathcal{R}}, \qquad (4.1)$$

where the choice of scale factors is left open. The scaling makes the size of the changes relative to the particular problem of interest. The scaling used in equations (3.1-3.3) is

$$\mathcal{A} = \|A\|_2, \qquad \mathcal{B} = \|b\|_2, \qquad \mathcal{R} = \|r\|_2.$$
(4.2)

Some authors prefer to measure the residual relative to b by choosing $\mathcal{R} = ||b||_2$. Other authors have no scaling, $\mathcal{A} = \mathcal{B} = \mathcal{R} = 1$. All of these cases are accommodated by the notation in equation (4.1). The effect of the choice for \mathcal{R} is discussed in section 6.1.

4.2. Notation. The formula for the Jacobian matrix $J_r(b)$ of the residual $r = [I - A(A^tA)^{-1}A^t]b$ with respect to b is clear.¹⁰ For derivatives with respect to the entries of A,

¹⁰The notation of section 2.2 would introduce a name, f_2 , for the function by which r varies with b when A is held fixed, $r = f_2(b)$, so that the notation for the Jacobian matrix is then $J_{f_2}(b)$. This pedantry will be discarded here to write $J_r(b)$ for the matrix of partial derivatives of r with respect to b with A held fixed.

it is necessary to use the "vec" construction to order the matrix entries into a column vector; vec(B) is the column of entries $B_{i,j}$ with i, j in co-lexicographic order.¹¹ The first order approximation (2.5) is then

$$\Delta r = J_r[\operatorname{vec}(A)]\operatorname{vec}(\Delta A) + J_r(b)\Delta b + \text{higher order terms in }\Delta A \text{ and }\Delta b$$
(4.3)

and upon taking norms

$$\|\Delta r\|_{\mathcal{R}} \leq \|J_r[\operatorname{vec}(A)]\operatorname{vec}(\Delta A)\|_{\mathcal{R}} + \|J_r(b)\Delta b\|_{\mathcal{R}} + o(\dots)$$

$$\leq \underbrace{\|J_r[\operatorname{vec}(\Delta A)]\|}_{\chi_r(A)} \|\Delta A\|_{\mathcal{A}} + \underbrace{\|J_r(b)\|}_{\chi_r(b)} \|\Delta b\|_{\mathcal{B}} + o(\dots)$$
(4.4)

where the norms of the two Jacobian matrices are induced from $\|\cdot\|_{\mathcal{R}}$, $\|\cdot\|_{\mathcal{A}}$ and from $\|\cdot\|_{\mathcal{R}}$, $\|\cdot\|_{\mathcal{B}}$, respectively. The high order term in equation (4.4) is $o(\max\{\|\Delta A\|_{\mathcal{A}}, \|\Delta b\|_{\mathcal{B}}\})$ because from equation (2.2) the norm $\max\{\|\cdot\|_{\mathcal{A}}, \|\cdot\|_{\mathcal{B}}\}$ has been given to the space that jointly consists of matrices A and vectors b.

4.3. Condition number of r with respect to b. For the orthogonal projection P defined in section 3.1, from r = (I - P)b follows $J_r(b) = I - P$, hence

$$\|J_r(b)\| = \max_{\Delta b} \frac{\|J_r(b)\Delta b\|_{\mathcal{R}}}{\|\Delta b\|_{\mathcal{B}}} = \max_{\Delta b} \frac{\left(\frac{\|(I-P)\Delta b\|_2}{\mathcal{R}}\right)}{\left(\frac{\|\Delta b\|_2}{\mathcal{B}}\right)} = \frac{\mathcal{B}}{\mathcal{R}},$$
(4.5)

which is equation (3.2) for the choice of scale factors in equation (4.2).

4.4. Condition number of r with respect to A. Evaluating the condition number of the residual requires a formula for the Jacobian matrix $J_r[vec(A)]$. Differentiating the entries of

$$r = \left[I - A \left(A^t A\right)^{-1} \!\! A^t\right] \! b$$

by those of A seems to be a daunting task. Instead, $J_r[vec(A)]$ is constructed from the total differential of the identity,

$$\begin{bmatrix} I & A \\ A^t & 0 \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} - \begin{bmatrix} b \\ 0 \end{bmatrix} = 0.$$

Assuming b is fixed because it already has been treated in section 4.3, the total differential is

$$\begin{bmatrix} I & A \\ A^t & 0 \end{bmatrix} \begin{bmatrix} dr \\ dx \end{bmatrix} + \begin{bmatrix} x_1 I & x_2 I & \cdots & x_n I \\ e_1 r^t & e_2 r^t & \cdots & e_n r^t \end{bmatrix} \operatorname{vec}(dA) = 0,$$

where x_i is the *i*-th entry of x and where e_i is the *i*-th column of the $n \times n$ identity matrix. Hence

$$\begin{bmatrix} dr \\ dx \end{bmatrix} = -\begin{bmatrix} I & A \\ A^t & 0 \end{bmatrix}^{-1} \begin{bmatrix} x_1 I & x_2 I & \cdots & x_n I \\ e_1 r^t & e_2 r^t & \cdots & e_n r^t \end{bmatrix} \operatorname{vec}(dA)$$
$$= -\begin{bmatrix} I - P & A(A^t A)^{-1} \\ (A^t A)^{-1} A^t & -(A^t A)^{-1} \end{bmatrix} \begin{bmatrix} x_1 I & x_2 I & \cdots & x_n I \\ e_1 r^t & e_2 r^t & \cdots & e_n r^t \end{bmatrix} \operatorname{vec}(dA)$$
$$= \begin{bmatrix} J_r[\operatorname{vec}(A)] \\ J_x[\operatorname{vec}(A)] \end{bmatrix} \operatorname{vec}(dA)$$
(4.6)

¹¹The alternative to placing the entries of matrices into column vectors is to use more general linear spaces and the Fréchet derivative. That approach seems unnecessarily abstract because the spaces have finite dimension.

in which $P = A(A^t A)^{-1}A^t$ is the orthogonal projection into the column space of A. The two matrix blocks in equation (4.6) are the Jacobian matrices of r and x as functions of the entries of A with b held fixed.

4.5. Transpose formula for condition numbers. The desired condition number is the norm induced from the norms in equation (4.1).

$$\|J_r[\operatorname{vec}(A)]\| = \max_{\Delta A} \frac{\|J_r[\operatorname{vec}(A)]\operatorname{vec}(\Delta A)\|_{\mathcal{R}}}{\|\operatorname{vec}(\Delta A)\|_{\mathcal{A}}}$$
$$= \frac{\mathcal{A}}{\mathcal{R}} \max_{\Delta A} \frac{\|J_r[\operatorname{vec}(A)]\operatorname{vec}(\Delta A)\|_2}{\|\Delta A\|_2}$$

The numerator and denominator are vector and matrix 2-norms, respectively. If A is an $m \times n$ matrix, then this maximization is a large problem with mn degrees of freedom. The identity for the norm of the transposed operator can be applied to reduce the degrees to m,

$$\|J_{r}[\operatorname{vec}(A)]\| = \frac{\mathcal{A}}{\mathcal{R}} \max_{\Delta r} \frac{\|J_{r}[\operatorname{vec}(A)]^{t} \Delta r\|_{2}^{*}}{\|\Delta r\|_{2}^{*}}.$$
(4.7)

Here, the identical norm for the transposed Jacobian matrix is induced from the duals of the 2-norms for matrices and vectors. The vector 2-norm is its own dual. The dual of the matrix 2-norm is determined in Grcar (2009) to be the sum of the singular values of the matrix, including multiplicities. This norm is sometimes called the nuclear norm or the trace norm.

4.6. Condition number of r with respect to A, continued. The application of equation (4.7) requires the evaluation of the matrix-vector product in the numerator. Note that for any vectors r' and x',

$$\begin{bmatrix} x_1 I & x_2 I & \cdots & x_n I \\ e_1 r^t & e_2 r^t & \cdots & e_n r^t \end{bmatrix}^t \begin{bmatrix} r' \\ x' \end{bmatrix} = \operatorname{vec}[r' x^t + r (x')^t].$$

With this identity it is now possible to compute, from equation (4.6),

$$\begin{split} \{J_r[\operatorname{vec}(A)]\}^t \Delta r &= \begin{bmatrix} J_r[\operatorname{vec}(A)] \\ J_x[\operatorname{vec}(A)] \end{bmatrix}^t \begin{bmatrix} \Delta r \\ 0 \end{bmatrix} \\ &= -\begin{bmatrix} x_1 I & x_2 I & \cdots & x_n I \\ e_1 r^t & e_2 r^t & \cdots & e_n r^t \end{bmatrix}^t \begin{bmatrix} I - P & A(A^t A)^{-1} \\ (A^t A)^{-1} A^t & -(A^t A)^{-1} \end{bmatrix} \begin{bmatrix} \Delta r \\ 0 \end{bmatrix} \\ &= -\begin{bmatrix} x_1 I & x_2 I & \cdots & x_n I \\ e_1 r^t & e_2 r^t & \cdots & e_n r^t \end{bmatrix}^t \begin{bmatrix} (I - P) \Delta r \\ (A^t A)^{-1} A^t \Delta r \end{bmatrix} \\ &= \operatorname{vec}(u_1 v_1^t + u_2 v_2^t) \,, \end{split}$$

in which

$$u_1 = (I - P)\Delta r$$
 $v_1 = x$
 $u_2 = r$ $v_2 = (A^t A)^{-1} A^t \Delta r$. (4.8)

Thus equation (4.7) is the following optimization,

$$\|J_{r}[\operatorname{vec}(A)]\| = \frac{\mathcal{A}}{\mathcal{R}} \max_{\Delta r} \frac{\|u_{1}v_{1}^{t} + u_{2}v_{2}^{t}\|_{2}^{*}}{\|\Delta r\|_{2}}.$$
$$= \frac{\mathcal{A}}{\mathcal{R}} \max_{\|\Delta r\|_{2}=1} \|u_{1}v_{1}^{t} + u_{2}v_{2}^{t}\|_{2}^{*}.$$
(4.9)

For ease of notation, let $g(\Delta r)$ be the objective function in equation (4.9). In Grear (2009) it is shown that

$$g(\Delta r) = \sqrt{\|u_1\|_2^2 \|v_1\|_2^2 + \|u_2\|_2^2 \|v_2\|_2^2 + 2 \|u_1\|_2 \|v_1\|_2 \|u_2\|_2 \|v_2\|_2 \cos(\theta_u - \theta_v)}, \quad (4.10)$$

where θ_u is the angle between u_1 and u_2 , and θ_v is the angle between v_1 and v_2 , and both angles should be taken from 0 to π . Evaluating the maximum has two parts.

The first step shows Δr can be restricted so that $\cos(\theta_u - \theta_v) \ge 0$. The vector Δr always could be decomposed into a component in $\operatorname{col}(A)$ and a component orthogonal to this subspace. Let the component inside $\operatorname{col}(A)$ be a'. Further, the component outside can be decomposed into components parallel to r and orthogonal to r, say $\gamma r + r'$ for some coefficient γ . With these choices to express Δr ,

$$\Delta r = \gamma r + r' + a'$$
 where $a' \in \operatorname{col}(A)$, $r' \perp \operatorname{col}(A)$, $r' \perp r$

the vectors in equation (4.8) are

$$u_1 = \gamma r + r'$$
 $v_1 = x$
 $u_2 = r$ $v_2 = (A^t A)^{-1} A^t a'$

and the angles are

$$\cos(\boldsymbol{\theta}_{u}) = \frac{u_{1}^{t}u_{2}}{\|u_{1}\|_{2} \|u_{2}\|_{2}} = \frac{\gamma \|r\|_{2}}{\sqrt{\gamma^{2} \|r\|_{2}^{2} + \|r'\|_{2}^{2}}}$$
$$\cos(\boldsymbol{\theta}_{v}) = \frac{v_{1}^{t}v_{2}}{\|v_{1}\|_{2} \|v_{2}\|_{2}} = \frac{x^{t}(A^{t}A)^{-1}A^{t}a'}{\|x\|_{2} \|(A^{t}A)^{-1}A^{t}a'\|_{2}}$$

Thus the sign of γ affects only the angle θ_u in equation (4.10), so it can be chosen to place θ_u in the same quadrant as θ_v (either from 0 to $\pi/2$, or from $\pi/2$ to π) and hence $\cos(\theta_u - \theta_v) \ge 0$. This means the maximum of equation (4.7) can be restricted to those Δr for which

$$L(\Delta r) = \sqrt{\|u_1\|_2^2 \|v_1\|_2^2 + \|u_2\|_2^2 \|v_2\|_2^2} \le g(\Delta r) \le \|u_1\|_2 \|v_1\|_2 + \|u_2\|_2 \|v_2\|_2$$
(4.11)
= $U(\Delta r)$.

The second step chooses Δr to maximize the upper bound $U(\Delta r)$. As before, the vector Δr always can be decomposed into a component in col(A) and a component in the orthogonal complement. Without loss of generality, assume $\Delta r = \cos(\phi)r'' + \sin(\phi)a''$ where a'' and r'' are unit vectors in col(A) and the complement, respectively, and where the coefficients are determined by an angle ϕ between 0 and $\pi/2$.¹² The vectors in equation (4.8) for this representation of Δr are

$$u_1 = \cos(\phi)r''$$
 $v_1 = x$
 $u_2 = r$ $v_2 = \sin(\phi)(A^t A)^{-1}A^t a''.$

¹²The coefficients $\cos(\phi)$ and $\sin(\phi)$ are non-negative so the choice of ϕ does not affect the choice of sign needed for equation (4.11).

The largest $||v_2||_2$ occurs when a'' is a left singular vector for the smallest singular value of A, σ_{\min} , in which case $v_2 = (\sin(\phi)/\sigma_{\min}) a''$; altogether

$$U(\Delta r) = \cos(\phi) ||x||_2 + \sin(\phi) \frac{||r||_2}{\sigma_{\min}}$$

The maximum of this formula with respect to ϕ determines an optimal $\Delta r_{\rm bnd}$ where the upper bound is

$$U(\Delta r_{\rm bnd}) = \sqrt{\left(\frac{\|r\|_2}{\sigma_{\rm min}}\right)^2 + \|x\|_2^2} .$$
(4.12)

The maximum has been verified using Mathematica (Wolfram, 2003).

The formula in equation (4.12) is the maximum of the upper bounds, which is not to say it is the maximum of equation (4.7). The objective function g and the lower and upper bounds L and U, when evaluated at Δr_{bnd} and Δr_{max} , must be arranged as follows,

$$L(\Delta r_{\text{bnd}}) \stackrel{a}{\leq} g(\Delta r_{\text{bnd}}) \stackrel{b}{\leq} g(\Delta r_{\text{max}}) \stackrel{c}{\leq} U(\Delta r_{\text{max}}) \stackrel{d}{\leq} U(\Delta r_{\text{bnd}})$$

These inequalities have the following justifications: (a) equation (4.11), (b) choice of Δr_{max} , (c) equation (4.12), and (d) choice of Δr_{bnd} . Therefore equation (4.12) is an upper bound for the maximum. From the formula for $L(\Delta r)$ in equation (4.11), the upper bound is at most $\sqrt{2}$ times larger than a lower bound for the maximum. Note that to complete the limits and the condition number, these values must be scaled by the coefficient \mathcal{A}/\mathcal{R} in equation (4.7).

4.7. Summary of condition numbers.

THEOREM 4.1 (SPECTRAL CONDITION NUMBERS). For the full rank linear least squares problem with solution $x = (A^t A)^{-1} A^t b$ and residual r = b - Ax, and for the scaled norms in equation (4.1) with scale factors A, B, and R,

$$\chi_r(b) = \frac{\mathcal{B}}{\mathcal{R}},$$

$$\frac{1}{\sqrt{2}} \frac{\mathcal{A}}{\mathcal{R}} \sqrt{\left(\frac{\|r\|_2}{\sigma_{\min}}\right)^2 + \|x\|_2^2} \leq \chi_r(A) \leq \frac{\mathcal{A}}{\mathcal{R}} \sqrt{\left(\frac{\|r\|_2}{\sigma_{\min}}\right)^2 + \|x\|_2^2},$$
(4.13)

where σ_{\min} is the smallest singular value of A. These formulas simplify to those in section 3.2 for the choice of scale factors in equation (4.2).

Proof. Section 4.3 derives $\chi_r(b)$, and sections 4.4–4.6 derive the bounds on $\chi_r(A)$.

5. Comparison with published bounds.

5.1. The estimate of Wedin. Table 5.1 lists the condition number estimates in some textbook error bounds for the least squares residual. All the values exceed the upper estimate of theorem 4.1 to varying degrees.

The very early formula of Wedin (1973, p. 224, eqn 5.4) is also reported in the more recent textbook of Björck (1996, p. 30, eqn. 1.4.27). It is for perturbations only to A, that is for the choice $\Delta b = 0$, and for the choice of scale factors $\mathcal{A} = \mathcal{R} = 1$. The value exceeds the estimate in theorem 4.1 by at most the factor $\sqrt{2}$, so it is at most double the condition number. The other two values in Table 5.1 can be severe overestimates.

10

TABLE 5.1

Condition number estimates in textbook error bounds for the least squares residual. The full rank least squares problem is $\min_x \|b - Ax\|_2$, the solution is x, the residual is r, the smallest nonzero singular value of A is σ_{\min} , the condition number of A is $\kappa_2 = \|A\|_2 / \sigma_{\min}$.

	norms and scale factors			maximum overestimation factor	
source	data		residual	estimate for $\chi_r(A)^{**}$	
Wedin (1973, p. 224, eqn. 5.4), Björck (1996, p. 30, eqn. 1.4.27)	$\ \Delta A\ _2$ $\mathcal{A} = 1$	$\Delta b = 0$	$\ \Delta r\ _2$ $\mathcal{R} = 1$	$\frac{\ r\ _2}{\sigma_{\min}} + \ x\ _2$	2
Stewart (1977, p. 655), Stewart and Sun (1990, p. 160, sec. 5.2)	$\ \Delta A\ _2$ $\mathcal{A} = 1$	$\Delta b = 0$	$\ \Delta r\ _2$ $\mathcal{R} = 1$	$\frac{\ b\ _2}{\sigma_{\min}}$	$\sqrt{2} \kappa_2$
Golub and Van Loan (1996, p. 242, eqn. 5.3.9), Higham (2002, p. 382, eqn. 20.2)**	$\max\left\{\frac{\ \Delta A\ _2}{\ A\ _2}, \frac{\ \Delta b\ _2}{\ b\ _2}\right\}$ $\mathcal{A} = \ A\ _2 \mathcal{B} = \ b\ _2$		$\frac{\ \Delta r\ _2}{\ b\ _2}$ $\mathcal{R} = \ b\ _2$	$2 \frac{\ A\ _2}{\sigma_{\min}} + 1^{**}$	κ_2
Theorem 4.1, equation (4.13)	$\frac{\ \Delta A\ _2}{\mathcal{A}}$	$\Delta b = 0$	$\frac{\ \Delta r\ _2}{\mathcal{R}}$	$\frac{\mathcal{A}}{\mathcal{R}}\sqrt{\left(\frac{\ r\ _2}{\sigma_{\min}}\right)^2 + \ x\ _2^2}$	$\sqrt{2}$

** The formula of Golub and van Loan and of Higham amounts to an estimate for $\chi_r(A) + \chi_r(b)$ and is compared against the sum of $\chi_r(b)$ and the tight estimate for $\chi_r(A)$. See section 5.3.

5.2. The estimate of Stewart. The value of Stewart (1977, p. 655) is also reported by Stewart and Sun (1990, p. 160, sec. 5.2). It again is for choices $\Delta b = 0$ and $\mathcal{A} = \mathcal{R} = 1$. Some assembly is required. Let $B = A + \Delta A$ be the perturbed matrix. Assume $\|\Delta A\|_2 < \sigma_{\min}$ so that *B* also has full rank.

For any matrix M, let $P_M = MM^{\dagger}$ be the orthogonal projection into the column space of M. With $\Delta b = 0$ the difference between the residuals of the original and the perturbed problems (1.1, 3.5) is $\Delta r = (I - P_B)b - (I - P_A)b$ so it is always true that

$$\|\Delta r\|_2 \le \|P_A - P_B\|_2 \|b\|_2.$$
(5.1)

Stewart (1977, p. 655) remarks that $||P_A - P_B||_2$ is to be bounded by applying an earlier result. He does not intend $||P_A - P_B||_2 < 1$ (p. 651, eqn. 4.1) which converts equation (5.1) into the useless $||\Delta r||_2 < ||b||_2$. Stewart means a complicated expression that introduces $||\Delta A||_2$ into the bound. This expression requires some preparation that is more easily followed in the presentation of Stewart and Sun (1990, pp. 160, 153, 148, 137).

Continuing the assembly of the bound, let the singular value decomposition of A be

$$\begin{bmatrix} U_1 & U_2 \end{bmatrix}^t A V = \begin{bmatrix} A_1 \\ 0 \end{bmatrix}$$

where $[U_1, U_2]$ and V are square orthonormal matrices and where A_1 is the square diagonal matrix of singular values. Let the corresponding factorization of ΔA be (Stewart and Sun, 1990, p. 137)

$$\begin{bmatrix} U_1 & U_2 \end{bmatrix}^t \Delta AV = \begin{bmatrix} E_1 \\ E_2 \end{bmatrix}$$

where $||E_i||_2 \le ||\Delta A||_2$ for i = 1, 2. Stewart and Sun (1990, p. 148) define

$$\hat{\kappa} = ||A||_2 ||(A_1 + E_1)^{-1}||_2$$

From the triangle inequality and from the Neumann series expansion for $(A_1 + E_1)^{-1}$,

$$| ||A_1^{-1}||_2 - ||(A_1 + E_1)^{-1}||_2 | \le ||A_1^{-1} - (A_1 + E_1)^{-1}||_2 \le \mathcal{O}(||\Delta A||_2^2).$$

These last two equations combine to

$$\hat{\kappa} = \|A\|_2 \,\sigma_{\min}^{-1} + \mathcal{O}(\|\Delta A\|_2^2) \,. \tag{5.2}$$

The final step applies a bound that requires some further hypotheses. For any matrix M, similar to $P_M = MM^{\dagger}$, let $R_M = P_{M^t} = (M^{\dagger}M)^t$ be the orthogonal projection into the row space of M (viewing the rows as column vectors). Since $B^{\dagger} = (B^t B)^{-1} B^t$ is a continuous function of ΔA , therefore both $BB^{\dagger} - AA^{\dagger}$ and $B^{\dagger}B - A^{\dagger}A$ converge to 0 as ΔA approaches 0.¹³ If $\|\Delta A\|_2$ is sufficiently small that both $\|P_A - P_B\|_2 \le 1$ and $\|R_A - R_B\|_2 \le 1$, then it can be shown (Stewart and Sun, 1990, p. 153, eqn. 4.1)

$$\|P_A - P_B\|_2 \le \frac{\hat{\kappa} \|E_2\|_2 / \|A\|_2}{\left[1 + (\hat{\kappa} \|E_2\|_2 / \|A\|_2)^2\right]^{1/2}}.$$
(5.3)

Altogether, combining equations (5.1–5.3) leaves

$$\|\Delta r\|_{2} \leq \frac{\|b\|_{2}}{\sigma_{\min}} \|\Delta A\|_{2} + \mathcal{O}(\|\Delta A\|_{2}^{2}), \qquad (5.4)$$

which is the bound from which the condition estimate in table 5.1 is taken.

The estimate for $\chi_r(A)$ in equation (5.4) can be obtained from theorem 4.1 by increasing the second term in the upper bound (4.13) by the factor V^2 ,

$$\sqrt{\left(\frac{\|r\|_2}{\sigma_{\min}}\right)^2 + \|x\|_2^2} \le \sqrt{\left(\frac{\|r\|_2}{\sigma_{\min}}\right)^2 + \mathbf{v}^2 \|x\|_2^2} = \sqrt{\frac{\|r\|_2^2 + \|Ax\|_2^2}{\sigma_{\min}^2}} = \frac{\|b\|_2}{\sigma_{\min}}$$

Consequently, Stewart and Sun's value can overestimate the upper bound for $\chi_r(A)$ by as much as V depending on circumstances. The worst situation is illustrated by the example of section 3.3 with $\phi = 0$ and $\beta \gg 1/\alpha$,

$$\frac{\frac{\|b\|_2}{\sigma_{\min}}}{\sqrt{\left(\frac{\|r\|_2}{\sigma_{\min}}\right)^2 + \|x\|_2^2}} = \frac{\frac{\sqrt{1+\beta^2}}{\alpha}}{\sqrt{\frac{1}{\alpha^2} + \beta^2 \cos^2(\phi) + \frac{\beta^2}{\alpha^2} \sin^2(\phi)}} = \frac{\sqrt{1+\beta^2}}{\sqrt{1+\alpha^2\beta^2}} \approx \frac{1}{\alpha} = \kappa_2.$$

5.3. The estimate of Golub and Van Loan and of Higham. The condition estimate of Golub and Van Loan (1996, p. 242, eqn. 5.3.9) and of Higham (2002, p. 382, eqn. 20.2) is for the choices $\Delta A \neq 0$ and $\Delta b \neq 0$ with the scale factors $\mathcal{A} = ||\mathcal{A}||_2$ and $\mathcal{R} = \mathcal{B} = ||b||_2$. They take the approach of equation (2.4) that uses a single quantity, ε , to measure the perturbations to A and b,

$$\begin{aligned} \|\Delta A\|_2 &\leq \varepsilon \|A\|_2 \\ \|\Delta b\|_2 &\leq \varepsilon \|b\|_2 \end{aligned} \right\} \quad \text{equivalently} \quad \varepsilon = \max\left\{\frac{\|\Delta A\|_2}{\|A\|_2}, \frac{\|\Delta b\|_2}{\|b\|_2}\right\}. \tag{5.5}$$

¹³Specific bounds on the norms of these differences can be derived from Wedin (1973, p. 221, thm. 4.1).

Since $\mathcal{B} = \mathcal{R}$, this approach can transform the bound (4.4) as follows,

$$\frac{\|\Delta r\|_{2}}{\mathcal{B}} \leq \|J_{r}[\operatorname{vec}(A)]\| \frac{\mathcal{A}}{\mathcal{B}} \frac{\|\Delta A\|_{2}}{\mathcal{A}} + \|J_{r}(b)\| \frac{\|\Delta b\|}{\mathcal{B}} + o(\varepsilon)$$
$$\leq \left[\|J_{r}[\operatorname{vec}(A)]\| \frac{\mathcal{A}}{\mathcal{B}} + \|J_{r}(b)\| \right] \varepsilon + o(\varepsilon)$$
$$= \left[\chi_{r}(A) + \chi_{r}(b) \right] \varepsilon + o(\varepsilon) .$$
(5.6)

From theorem 4.1 with the choices $\mathcal{R} = \mathcal{B} = ||b||_2$,

$$\chi_{r}(A) + \chi_{r}(b) \leq \left\{ \frac{\|A\|_{2}}{\|b\|_{2}} \sqrt{\left(\frac{\|r\|_{2}}{\sigma_{\min}}\right)^{2} + \|x\|_{2}^{2}} \right\} + 1$$
$$\leq \left\{ \frac{\|A\|_{2}}{\|b\|_{2}} \sqrt{\left(\frac{\|r\|_{2}}{\sigma_{\min}}\right)^{2} + \mathbf{v}^{2} \|x\|_{2}^{2}} \right\} + 1 = \kappa_{2} + 1.$$
(5.7)

Golub and Van Loan and Higham state a larger value, $2\kappa_2 + 1$.¹⁴ Since these formulas can be derived from the sum $\chi_r(A) + \chi_r(b)$ they are not joint condition numbers in the sense of equation (2.4). Moreover, the derivation inserts V into equation (5.7), so the result can overestimate the sum by as much as a factor of κ_2 . Close to the worst situation for the specific value $2\kappa_2 + 1$ of Golub, Van Loan and Higham is again illustrated by the example of section 3.3 with $\phi = 0$ and $\beta \gg 1/\alpha$,

$$\frac{2\kappa_2 + 1}{\left\{\frac{\|A\|_2}{\|b\|_2}\sqrt{\left(\frac{\|r\|_2}{\sigma_{\min}}\right)^2 + \|x\|_2^2}\right\} + 1} = \frac{\frac{2}{\alpha} + 1}{\left\{\frac{1}{\sqrt{1 + \beta^2}}\sqrt{\frac{1}{\alpha^2} + \beta^2}\right\} + 1} \approx \frac{1}{\alpha} = \kappa_2 \,.$$

Note the bound (5.7) is not sensitive to the angle θ between r and col(A) because of the choice for the scale factor $\mathcal{R} = ||b||_2$. Choices for \mathcal{R} are discussed in section 6.1.

6. Discussion.

6.1. Measuring perturbations to r relative to b. As mentioned in section 4.1, scaled changes to the residual are typically measured by choosing $\mathcal{R} = ||r||_2$ or $||b||_2$. The two cases are contrasted in Table 6.1. The choice $\mathcal{R} = ||b||_2$ makes it appear that θ is not a source of ill-conditioning because the sensitivity of r to A is masked by measuring changes to r against the always larger vector b. The choice $\mathcal{R} = ||r||_2$ measures perturbations relatively. The next section 6.2 describes a situation when the relative measure is appropriate.

6.2. Significance for iterative methods. Many iterative methods proceed by building orthogonal bases from the residuals of least squares projections. For example, for a symmetric matrix A and a unit vector v_1 , the Lanczos iteration

$$\beta_{j+1}v_{j+1} = Av_j - \alpha_j v_j - \beta_j v_{j-1}$$

produces a sequence of orthonormal vectors v_1, v_2, v_3, \ldots This algorithm can be viewed as repeatedly evaluating a residual $r_{j+1} = \beta_{j+1}v_{j+1}$ for either of two orthogonal projections:

¹⁴Their value resembles the $\sqrt{2} \kappa_2 + 1$ that was originally stated by Björck (1967, p. 16, eqn. 7.7).

TABLE 6.1

Effect of scaling on condition numbers for the least squares residual. The full rank least squares problem is $\min_x \|b - Ax\|_2$, the solution is x, the residual is r, $\kappa_2 = \|A\|_2 / \sigma_{\min}$ is the spectral matrix condition number of A, σ_{\min} is the smallest singular value of A, $\mathbf{V} = \|Ax\|_2 / (\|x\|_2 \sigma_{\min})$ is van der Sluis's ratio between 1 and κ_2 , and $\boldsymbol{\theta}$ is the angle between b and $\operatorname{col}(A)$.

norms and scale factors			condition numbers		
$\frac{\ \Delta A\ _2}{\mathcal{A}}$	$\frac{\ \Delta b\ _2}{\mathcal{B}}$	$\frac{\ \Delta r\ _2}{\mathcal{R}}$	tight estimate for $\chi_r(A)$	$\chi_r(b)$	
$\mathcal{A} = \ A\ _2$	$\mathcal{B} = \ b\ _2$	$\mathcal{R} = \ r\ _2$	$\kappa_2 \sqrt{1 + \left(\frac{\cot(\boldsymbol{\theta})}{\mathbf{v}}\right)^2}$	$\csc(\boldsymbol{\theta})$	
$\mathcal{A} = \ A\ _2$	$\mathcal{B} = \ b\ _2$	$\mathcal{R} = \ b\ _2$	$\kappa_2 \sqrt{\sin^2(\theta) + \left(\frac{\cos(\theta)}{v}\right)^2}$	1	

(1) the projection of Av_j into the span of v_{j-1} and v_j , or (2) the orthogonal projection of $A^j v_1$ into the Krylov subspace spanned by $v_1, Av_1, \ldots, A^{j-1}v_1$.

The appropriate scale factor for measuring perturbations to r_{j+1} is $\mathcal{R} = ||r_{j+1}||_2$. The relative error in r_{j+1} becomes the absolute error in the normalized vector, v_{j+1} , which continues the Lanczos iteration. In ideal circumstances the vectors v_{j-1} and v_j are close to orthonormal. If $A = [v_{j-1}, v_j]$ is an orthonormal matrix, then $\kappa_2 = \mathbf{v} = 1$ so the tight estimate in Table 6.1 simplifies to $\chi_r(A) \approx \csc(\theta) = \chi_r(b)$ where θ is the angle between $b = Av_j$ and $\operatorname{col}(A)$. Thus r_{j+1} is ill-conditioned when θ is small.

6.3. Condition numbers of orthogonal projections. In the least squares problem, the condition number of the orthogonal projection Ax is essentially that of the residual. In addition to equations (4.1, 4.2), it is necessary to specify the scaled norm for the projection:

$$\|\Delta(Ax)\| = \frac{\|\Delta(Ax)\|_2}{\mathcal{P}}$$
 where $\mathcal{P} = \|Ax\|_2$.

From Ax = Pb follows $J_{Ax}(b) = P$ hence $\chi_{Ax}(b) = \mathcal{B}/\mathcal{P}$. Since Ax = b - r so $J_{Ax}(A) = -J_r(A)$. With \mathcal{P} replacing \mathcal{R} in the formulas, the condition numbers of the orthogonal projection are

$$\chi_{Ax}(b) = \sec(\boldsymbol{\theta}),$$

$$\frac{1}{\sqrt{2}} \kappa_2 \sqrt{\tan^2(\boldsymbol{\theta}) + \frac{1}{\mathbf{v}^2}} \leq \chi_{Ax}(A) \leq \kappa_2 \sqrt{\tan^2(\boldsymbol{\theta}) + \frac{1}{\mathbf{v}^2}}$$

Both κ_2 and θ are independent sources of ill-conditioning.

6.4. Column transformations. The linear least squares residual is invariant with respect to transformations of the matrix columns, so there is reason to seek changes to the columns that might reduce the condition number of the residual. If A is replaced by AM for some nonsingular matrix M that makes AM an orthonormal matrix, then with the scale factors of equation (4.2) it has been noted in section 6.2 that the tight estimate is $\chi_r(AM) \approx \csc(\theta)$ which leaves only θ as a source of ill-conditioning.

A less costly transformation is M = D for a diagonal matrix D. Two reasons suggest choosing D to equilibrate the columns of AD. First, least squares problems typically are

solved using the QR factorization. The errors of that calculation can be accounted for by backward rounding errors whose relative size in each column is roughly the same across all columns (Higham, 2002, p. 385, thm. 20.3). Second, equilibrating the columns is approximately the optimal column scaling to reduce the matrix condition number (van der Sluis, 1969). Nevertheless, even if $\kappa_2(AD) \leq \kappa_2(A)$, the scaling also alters van der Sluis's ratio in equation (3.6), so it is unclear whether the net change to the condition number in equation (3.1) is for the better.

Acknowledgements. I thank the editor Prof. D. O'Leary and the three referees for corrections and suggestions that much improved this paper.

References.

- Å. Björck. Solving linear least squares problems by Gram-Schmidt orthogonalization. *BIT*, 7(1):1–21, 1967.
- Å. Björck. Numerical Methods for Least Squares Problems. SIAM, Philadelphia, 1996.
- A. J. Geurts. A contribution to the theory of condition. *Numer. Math.*, 39(1):85–96, June 1982.
- G. H. Golub and C. F. Van Loan. *Matrix Computations*. The Johns Hopkins University Press, Baltimore, 3rd edition, 1996.
- G. H. Golub and J. H. Wilkinson. Note on the iterative refinement of least squares solutions. *Numer. Math.*, 9(2):139–148, December 1966.
- S. Gratton. On the condition number of linear least squares problems in a weighted Frobenius norm. *BIT*, 36(3):523–530, September 1996.
- J. F. Grcar. Spectral condition numbers of full rank linear least squares solutions. Submitted. Available from the world wide web at arxiv.org as arXiv:1003.2733v3 [math.NA], 2009.
- N. J. Higham. Accuracy and Stability of Numerical Algorithms. SIAM, Philadelphia, 2nd edition, 2002.
- A. N. Malyshev. A unified theory of conditioning for linear least squares and Tikhonov regularization solutions. *SIAM J. Matrix Anal. Appl.*, 24:1186–1196, 2003.
- J. R. Rice. A theory of condition. SIAM J. Numer. Anal., 3(2):287-310, 1966.
- G. W. Stewart. On the perturbation of pseudo-inverses, projections and linear least squares problems. *SIAM Review*, 19(4):634–662, October 1977.
- G. W. Stewart and J.-G. Sun. *Matrix Perturbation Theory*. Academic Press, San Diego, 1990.
- L. N. Trefethen and D. Bau, III. Numerical Linear Algebra. SIAM, Philadelphia, 1997.
- A. van der Sluis. Condition numbers and equilibration of matrices. *Numer. Math.*, 14:14–23, 1969.
- A. van der Sluis. Stability of the solutions of linear least squares problems. *Numer. Math.*, 23:241–254, 1975.
- P.-A. Wedin. Perturbation theory for pseudo-inverses. BIT, 13(2):217–232, 1973.
- J. H. Wilkinson. *Rounding Errors in Algebraic Processes*. Prentice Hall, Englewood Cliffs, 1963.
- S. Wolfram. *The Mathematica Book*. Wolfram Media / Cambridge University Press, Champaign and Cambridge, 5th edition, 2003.