Error bounds for computed least squares estimators

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Abstract

This paper is concerned with normwise errors in the LS estimation for linear regression. It provides probabilistic tail bounds for the normwise error between the \textit{computed} least squares estimator and the parameter vector, when the least squares problem is solved in floating point arithmetic using either the normal equations method or a backward stable method (for example, using the Householder QR factorization or the singular value decomposition). These bounds are used to provide a condition under which the computationally more efficient normal equations method can safely be used instead of a backward stable method, without any loss of accuracy in the computed estimator.

\textit{Keywords: } Linear regression, Least squares, Perturbation theory, Rounding errors, Normwise error bounds, Probabilistic tail bounds

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1. Introduction

Consider the linear model

\[ \mathbf{y} = X\mathbf{\beta} + \mathbf{v}, \quad \mathbf{v} \sim \mathcal{N}(0, \sigma^2 I), \]  \hspace{1cm} (1)

where \( \mathbf{y} \) is an observation vector, \( X \in \mathbb{R}^{m \times n} \) is a model matrix with rank \( n \), \( \mathbf{\beta} \) is an unknown parameter vector, and \( \mathbf{v} \) is a random noise vector following
the normal distribution \( \mathcal{N}(0, \sigma^2 I) \). The goal of regression is to recover \( \beta \) given \( X \) and \( y \).

It is well known that the maximum likelihood estimator of \( \beta \) is given by the least squares (LS) solution,

\[
\beta_{\text{LS}} = \mathop{\arg\min}_z \| y - Xz \|_2, \tag{2}
\]

which satisfies the normal equations

\[
X^T X \beta_{\text{LS}} = X^T y. \tag{3}
\]

Hence,

\[
\beta_{\text{LS}} = X^\dagger y, \tag{4}
\]

where \( X^\dagger = (X^T X)^{-1} X^T \) is the Moore-Penrose generalized inverse of \( X \).

Statisticians are typically interested in the statistical properties of the error between the exact LS solution \( \beta_{\text{LS}} \) and the parameter vector \( \beta \) in (1). The basic properties of \( \beta_{\text{LS}} - \beta \) are well known, and we discuss some of these in the next section. In practice, however, \( \beta_{\text{LS}} \) cannot be computed exactly. Due to rounding errors that inevitably occur when working in floating point arithmetic, the \textit{computed} LS solution contains errors.

Several direct numerical methods can be used to compute the LS solution \( \beta_{\text{LS}} \), see, e.g., [1, Chapter 2] and [2, Chapter 5]. One method is the normal equations method. It explicitly forms the symmetric positive definite matrix \( X^T X \) and the vector \( X^T y \), and solves (3) using the Cholesky factorization of \( X^T X \). Other commonly used methods for computing \( \beta_{\text{LS}} \) perform a factorization of the matrix \( X \), such as the Householder QR factorization or the singular value decomposition (SVD), and use the computed factors to solve (2). These methods are \textit{backward stable}. (The precise definition of backward stability is given in Section 3.) We note that the SVD is particularly appropriate when \( X \) is rank deficient or nearly rank deficient, in which case a truncated SVD can be used as a form of regularization; see, e.g., [2, Section 5.5] or [3].

The normal equations method requires fewer floating point operations than any backward stable method. It is also more suitable for block/parallel compu-
tations and requires less CPU time than any backward stable method, especially when $m \gg n$. By any measurable standard, the normal equations method is the most efficient option for solving the LS problem \cite{2}. For further discussion of performance comparisons, see, e.g., \cite{4}, Sections 3.2 & 3.6. Nowadays, even for moderate size LS problems one can quickly compute the solution using any of the above methods. But in some applications, such as wireless communications, one may need to solve many LS problems of small or moderate size as quickly as possible to reduce the latency. Thus computational efficiency is still crucial for small or moderate size problems in some applications.

In theory all of these methods produce the LS solution $\beta_{LS}$. However, the accuracy of these methods when implemented in finite precision arithmetic can be very different. We use $\tilde{\beta}_N$ and $\tilde{\beta}_B$ to denote the LS solutions computed in floating point arithmetic via the normal equations method or a backward stable method, respectively.

Numerical analysts are concerned with the normwise errors between the exact and computed LS solutions: $\|\tilde{\beta}_N - \beta_{LS}\|_2$ and $\|\tilde{\beta}_B - \beta_{LS}\|_2$. Typically $\tilde{\beta}_B$ is at least as accurate as and can be much more accurate than $\tilde{\beta}_N$ in terms of the above measure when the least squares residual $\|y - X\beta_{LS}\|_2$ is small. For some numerical comparisons, see, e.g., \cite{2}, p268 or \cite{5}, p358.

To summarize, there is an efficiency vs accuracy tradeoff between the normal equations method and backward stable methods for solving \cite{2}.

Contributions

In practice, a user may be interested in the error between the computed LS solution and the parameter vector $\beta$ in \cite{1}. In this paper, we fill a gap in the literature by providing probabilistic tail bounds on $\|\tilde{\beta}_N - \beta\|_2$ and $\|\tilde{\beta}_B - \beta\|_2$. We believe that our new bounds, which take into account both the probabilistic nature of the problem \cite{1} as well as the rounding error properties of the numerical methods, will be a useful reference in applications.

Additionally, we use our bounds to provide a condition under which the normal equations method can be used instead of a backward stable method,
without any loss of accuracy in the computed estimator. We believe that such a condition will be helpful to a user who wishes to use the most computationally efficient method for linear regression, as long as this can be done without compromising any accuracy with respect to the parameter vector $\beta$ in the linear model.

**Notation**

We use uppercase letters for matrices, and lowercase letters for vectors and scalars. $I$ is the identity matrix. $\|M\|_2$, $\|M\|_F$, and $M^\dagger$ are, respectively, the spectral norm, Frobenius norm, and Moore-Penrose generalized inverse of the matrix $M$. The *stable rank* of $M$ is defined as $r = \|M\|_F^2/\|M\|_2^2$. See for example [6] for several applications of the stable rank.

Bold font denotes a random variable. $E\{\mu\}$ and $V\{\mu\}$ are the mean and variance of the random variable $\mu$. By $\mathbf{y} \sim \mathcal{N}(v, B)$ we mean that $\mathbf{y}$ follows a multivariate normal distribution with mean $v$ and covariance matrix $B$, and by $\mathbf{\omega} \sim \chi^2(k)$ we mean that $\mathbf{\omega}$ follows a chi-squared distribution with $k$ degrees of freedom.

$\text{Prob}\{x\}$ denotes the probability of event $x$. We will provide *probabilistic tail bounds* of the form

$$\text{Prob}\{\mu > c\} \leq f(\tau), \quad \text{Prob}\{\mu < c/\tau\} \leq g(\tau),$$

(5)

for a given $c$ and $\tau > 1$. If $f(\tau)$ (respectively, $g(\tau)$) decays very quickly to zero with increasing $\tau$, then the random variable $\mu$ is very unlikely to be much larger (respectively, smaller) in magnitude than $c$. How unlikely this is, precisely, is quantified by $f(\tau)$ and $g(\tau)$.

**Related problems**

We briefly mention that when the matrix $X$ is large and sparse, using an iterative method (such as LSQR [7] or LSQR [8]) is often an appropriate option for solving the LS problem (2). Additionally, if the model matrix $X$ is also subject to noise, i.e.,

$$\mathbf{y} = (X + \mathbf{E})\beta + \mathbf{v}, \quad \mathbf{v} \sim \mathcal{N}(0, \sigma_v^2 I), \quad \text{vec}(\mathbf{E}) \sim \mathcal{N}(0, \sigma_E^2 I),$$

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then it may be more appropriate to solve a scaled total least squares (STLS) problem instead of a LS problem (2). The STLS solution can be computed using the SVD of the augmented matrix \([y, X]\). In this paper we focus on direct methods for the LS problem (2), and refer readers interested in STLS to [3].

2. Statistical properties the exact LS estimator

In this section we provide some statistical properties of some quantities associated with the exact LS estimator.

First we consider the error \(\beta_{ls} - \beta\). From (1) and (3), it follows that

\[
\beta_{ls} - \beta = X^T y - X^T (y - \nu) = X^T \nu \sim N(0, \sigma^2 (X^T X)^{-1}).
\]

As we are interested in the normwise error, we consider

\[
\|\beta_{ls} - \beta\|_2^2 = \|X^T \nu\|_2^2.
\]

It is straightforward to verify that the above is a linear combination of independent chi-squared variables with 1 degree of freedom. Consider the singular value decomposition (SVD) of \(X\):

\[
X = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} S \end{bmatrix} V^T = U_1 S V^T,
\]

where \(U = [U_1, U_2] \in \mathbb{R}^{m \times m}\) and \(V \in \mathbb{R}^{n \times n}\) are orthogonal matrices, and \(S = \text{diag}(\sigma_1, \ldots, \sigma_n)\) with

\[
\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \equiv \sigma_{\min} > 0
\]

the singular values of \(X\). Then

\[
\|\beta_{ls} - \beta\|_2^2 = \|VS^{-1}U_1^T \nu\|_2^2 = \sum_{i=1}^{n} \frac{\sigma_i^2}{\sigma_i} \omega_i^2,
\]

where \(w = \sigma^{-1} U_1^T \nu \sim N(0, I)\) so the elements \(\omega_i\) of \(w\) are independent and satisfy \(\omega_i^2 \sim \chi^2(1)\).
Rust uses (10) to show that the mean squared error is bounded by
\[ E\{ \| \beta_{LS} - \beta \|_2^2 \} \leq \frac{n\sigma^2}{\sigma_{\min}^2}. \]

More precisely, from (10) we have
\[ E\{ \| \beta_{LS} - \beta \|_2^2 \} = \sum_{i=1}^{n} \frac{\sigma^2}{\sigma_i^2} E\{ \omega_i^2 \} = \sum_{i=1}^{n} \frac{\sigma^2}{\sigma_i^2} = \sigma^2 \| X^\top \|=^2_F, \tag{10} \]
and
\[ V\{ \| \beta_{LS} - \beta \|_2^2 \} = \sum_{i=1}^{n} \frac{\sigma_i^4}{\sigma_i^2} V\{ \omega_i^2 \} = 2 \sum_{i=1}^{n} \frac{\sigma_i^4}{\sigma_i^2}. \tag{11} \]

Besides the mean and variance, it is also possible to obtain tail bounds on the normwise least squares error (10). Several properties of linear combinations of independent chi-squared random variables have been documented, see, e.g., [11].

More recently, probabilistic tail bounds have appeared in the literature. Below we state one such result that follows directly from [12, Theorem 3.1]. Other related results can be found in [13, 14].

**Lemma 1.** Let \( M \in \mathbb{R}^{p \times q} \) be a nonzero deterministic matrix with stable rank \( r = \| M \|_F^2/\| M \|_F^2 \), and let \( v \sim N(0, \sigma^2 I) \). For any \( \tau > 1 \),
\[ \text{Prob}\{ \| Mv \|_2 > \tau \sigma \| M \|_F \} \leq \exp \left( -\frac{r}{2} (\tau - 1)^2 \right) \tag{12} \]
and
\[ \text{Prob}\left\{ \| Mv \|_2 < \frac{\sigma \| M \|_F}{\tau} \right\} \leq \exp \left( -\frac{r}{4} \frac{\tau^2 - 1}{\tau^4} \right). \tag{13} \]

Note that the bound in (12) decreases to 0 exponentially with increasing \( \tau \) and \( r \). On the other hand, the bound in (13) does not decrease to 0 with increasing \( \tau \), but, like (12), does decrease to 0 with increasing \( r \). Thus, as explained after (10), it is very unlikely that \( \| Mv \|_2 \) is much larger than \( \sigma \| M \|_F \), and it is very unlikely that \( \| Mv \|_2 \) is much smaller than \( \sigma \| M \|_F \) unless \( r \) is close to its lower bound 1.

For example, take \( \tau = 5 \). Suppose \( M \) has stable rank \( r = 100 \). Then both inequalities \( \| Mv \|_2 > 5 \sigma \| M \|_F \) and \( \| Mv \|_2 < (1/5) \sigma \| M \|_F \) hold with probability less than \( 10^{-10} \), so \( \| Mv \|_2 \) is extremely likely to be within a factor 5
of $\| M \|_F$. On the other hand, if $M$ has stable rank $r = 2$, $\| M v \|_2 > 5\sigma \| M \|_F$ holds with probability less than $10^{-8}$ but $\| M v \|_2 < (1/5)\sigma \| M \|_F$ holds with probability less than only 0.63.

With Lemma 1, we can show the following theorem.

**Theorem 1.** Consider the normwise error between the parameter vector $\beta$ in the linear model (1) and the LS solution $\beta_{LS}$ defined in (4). For any $\tau > 1$,

$$\text{Prob}\{ \| \beta_{LS} - \beta \|_2 > \tau \sigma \| X^\dagger \|_F \} \leq \exp\left( -\frac{1}{2} \frac{\| X^\dagger \|_F^2}{\| X^\dagger \|_2^2} \left( \tau - 1 \right)^2 \right)$$

(14)

$$\leq \exp\left( -\frac{1}{2} \left( \tau - 1 \right)^2 \right)$$

(15)

and

$$\text{Prob}\{ \| \beta_{LS} - \beta \|_2 < \frac{\sigma \| X^\dagger \|_F}{\tau} \} \leq \exp\left( -\frac{1}{4} \frac{\| X^\dagger \|_F^2}{\| X^\dagger \|_2^2} \left( \frac{\tau^2 - 1}{\tau^4} \right)^2 \right)$$

(16)

$$\leq \exp\left( -\frac{1}{4} \left( \frac{\tau^2 - 1}{\tau^4} \right)^2 \right).$$

(17)

**Proof.** Recall from (1) that $\| \beta_{LS} - \beta \|_2 = \| X^\dagger v \|_2$. Thus, (14) and (15) follow directly from Lemma 1 by setting $M = X^\dagger$. Replacing the stable rank $\| X^\dagger \|_F^2/\| X^\dagger \|_2^2$ in (14) and (15) by its lower bound 1 leads to (16) and (17), respectively, which are weaker but independent of $X$. \qed

Comments analogous to those after Lemma 1 also apply here. The bound (16) decreases to 0 very fast with increasing $\tau$. Thus, it is always extremely unlikely that $\| \beta_{LS} - \beta \|_2$ is much larger than its expected value, $\sigma \| X^\dagger \|_F$. The bound (17) does not tend to 0 with increasing $\tau$ but it is small unless $\| X^\dagger \|_F/\| X^\dagger \|_2$ is close to its lower bound 1. Thus, if the stable rank of $X^\dagger$ is not close to 1 (say $\| X^\dagger \|_F \geq 10 \| X^\dagger \|_2$) then it is extremely unlikely that $\| \beta_{LS} - \beta \|_2$ is much smaller than $\sigma \| X^\dagger \|_F$. However, if the matrix $X$ has one singular value that is very small compared to the other $n - 1$ singular values, so $\| X^\dagger \|_F \approx \| X^\dagger \|_2$, then it is not so unlikely that $\| \beta_{LS} - \beta \|_2$ is much smaller than $\sigma \| X^\dagger \|_F$.

We can conclude from Theorem 1 that unless $\| X^\dagger \|_F/\| X^\dagger \|_2$ is very close to 1, the relative error $\frac{\| \beta_{LS} - \beta \|_2}{\| \beta \|_2}$ is very likely to be close to $\frac{\sigma \| X^\dagger \|_F}{\| \beta \|_2}$. If this
relative error is not smaller than 1, then the exact LS solution $\beta_{LS}$ will have
almost no accurate digits compared to the parameter vector $\beta$. Thus, if

$$\frac{\sigma\|X^\dagger\|_F}{\|\beta\|_2} \geq 1,$$

(18)

there is not much point to solving the LS problem (2), regardless of the method
used. Note that (18) can be rewritten as

$$\kappa_F(X) \geq \frac{\|X\|_F\|\beta\|_2}{\sigma},$$

where the right hand side can be interpreted as the signal-to-noise ratio (SNR)
of the linear model (2). Thus when the condition number is larger than the SNR,
one may need to obtain more accurate measurements, redesign the model (2),
or apply a regularized LS method instead.

In practice, a condition number estimator can be used to estimate $\kappa_F(X)$
if it not known from the application context; see for example [3, chapter 14].
Another difficulty in checking (18) in practice is that $\|\beta\|_2$ is unknown. But we
will provide a practical strategy for estimating $\|\beta\|_2$ in Section 4.

We can also use Lemma 2 to establish tail bounds on the norm of the exact
LS residual vector, $\rho_{LS} = y - X\beta_{LS}$. If $m = n$ then $\rho_{LS} = 0$. Now suppose that
$m > n$. From (3) and (4),

$$\rho_{LS} = y - X\beta_{LS} = (I - XX^\dagger)y = (I - XX^\dagger)v = U_2U_2^T v,$$

(19)

where $U_2 \in \mathbb{R}^{m \times (m-n)}$ with orthonormal columns is defined in the SVD of $X$
in (3) and $v \sim N(0, \sigma^2 I)$ is the noise in the linear model (2).

With $w = \sigma^{-1}U_2^Tv \sim N(0, I)$, the random variable $\|\rho_{LS}\|^2/\sigma^2$ follows a
chi-squared distribution with $m - n$ degrees of freedom:

$$\frac{\|\rho_{LS}\|^2}{\sigma^2} = \frac{\|U_2^Tv\|^2}{\sigma^2} = \sum_{i=1}^{m-n} \omega_i^2 \sim \chi^2(m - n).$$

(20)

Thus, analogously to (10) and (11),

$$\mathbb{E}\{\|\rho_{LS}\|^2\} = \sigma^2(m - n), \quad \forall \{\|\rho_{LS}\|^2\} = 2\sigma^4(m - n).$$

Below we provide a tail bound for the exact LS residual that is analogous to the
one given in Theorem 1.
**Theorem 2.** Suppose that $X \in \mathbb{R}^{m \times n}$ with $m > n$ in the linear model (11). For any $\tau > 1$, the exact LS residual $\mathbf{r}_{LS} = U_2 U_2^T \mathbf{v}$ in (11) satisfies

$$\operatorname{Prob}\{ \| \mathbf{r}_{LS} \|_2 > \tau \sigma \sqrt{m-n} \} \leq \exp \left( -\frac{m-n}{2} \left( \tau - 1 \right)^2 \right)$$

and

$$\operatorname{Prob}\{ \| \mathbf{r}_{LS} \|_2 < \frac{\sigma \sqrt{m-n}}{\tau} \} \leq \exp \left( -\frac{m-n}{4} \frac{\left( \tau^2 - 1 \right)^2}{\tau^4} \right).$$

**Proof.** The result follows directly from Lemma 1 by setting $M = U_2 U_2^T$, so that

$$\| M \|_F = \| U_2 U_2^T \|_F = \sqrt{m-n}, \quad \| M \|_2 = \| U_2 U_2^T \|_2 = 1. \quad \square$$

Comments analogous to those after Lemma 1 also apply here. It is always extremely unlikely that $\| \mathbf{r}_{LS} \|_2$ is much larger than its expected value, $\sigma \sqrt{m-n}$.

If $m$ is not very close to $n$ (say $m \gtrsim n + 40$) then it is also very unlikely that $\| \mathbf{r}_{LS} \|_2$ is much smaller than $\sigma \sqrt{m-n}$. However, if the matrix $X$ is almost square, then it is not so unlikely that $\| \mathbf{r}_{LS} \|_2$ is much smaller than $\sigma \sqrt{m-n}$.

**3. Error in the computed LS solutions**

In the analysis in the previous section, $\hat{\beta}_{LS}$ is the exact least squares solution. Due to rounding errors that inevitably occur when working in floating point arithmetic, the computed LS solution has errors.

It is well known (see for example [2, chapter 5] and [3, chapter 20]) that the computed LS solution obtained by the normal equations method satisfies

$$\tilde{\beta}_N = (X^T X + \Delta M)^{-1} (X^T y + \Delta c),$$

$$\| \Delta M \|_2 \leq \epsilon \| X \|_2^2, \quad \| \Delta c \|_2 \leq \epsilon \| X \|_2 \| y \|_2, \quad (21)$$

while the computed LS solution obtained by a backward stable method (for example, via the Householder QR factorization or the SVD) satisfies

$$\tilde{\beta}_B = (X + \Delta X)^T (y + \Delta y),$$

$$\| \Delta X \|_2 \leq \epsilon \| X \|_2, \quad \| \Delta y \|_2 \leq \epsilon \| y \|_2. \quad (22)$$
In the above, $\epsilon$ is a multiple of the machine unit roundoff, which is approximately $10^{-16}$ in IEEE double precision. Note that $\boldsymbol{\beta}_n$ is the exact solution of a ‘nearby’ LS problem, $\min_z \| (y + \Delta y) - (X + \Delta X) z \|_2$.

Using (21) and (22), it is possible to bound the error between the exact and computed LS solutions. Such bounds are well known and can be found, e.g., in [2, chapter 5] or [3, chapter 20]. Our purpose, however, is to bound the error between the parameter vector in the linear model (1) and the computed LS solution, analogous to those in the previous section involving the exact LS solution. We will need the following lemma.

**Lemma 2.** The noise $\mathbf{v}$ in the linear model (11) satisfies

$$E\{\| \mathbf{v} \|_2 \} \leq \sqrt{E\{\| \mathbf{v} \|_2^2 \}} = \sigma \sqrt{m},$$

and for any $\tau > 1$,

$$\text{Prob}\{\| \mathbf{v} \|_2 > \tau \sigma \sqrt{m} \} \leq \exp \left( -\frac{m}{2} (\tau - 1)^2 \right).$$

**Proof.** As $\mathbf{v} \sim \mathcal{N}(0, \sigma^2 I)$,

$$\frac{\| \mathbf{v} \|_2^2}{\sigma^2} \sim \chi^2(m),$$

from which (23) immediately follows. The bound (24) can be obtained by setting $M = I$ in Lemma 1.

The following theorem applies when the LS solution is computed by the normal equations.

**Theorem 3.** Let $\kappa_2(X) = \| X \|_2 \| X^\dagger \|_2$ and suppose $\epsilon \kappa_2^2(X) < 1$. The relative normwise error between the parameter vector $\beta$ in the linear model (11) and the computed LS solution $\tilde{\beta}_n$ obtained by the normal equations method satisfies

$$\frac{\| \tilde{\beta}_n - \beta \|_2}{\| \beta \|_2} \leq 2 \kappa_2^2(X) \frac{(1 + \kappa_2(X) \epsilon) \kappa_2(X)}{1 - \epsilon \kappa_2^2(X)} \frac{\| \mathbf{v} \|_2}{\| \beta \|_2}$$

and

$$E\left\{ \frac{\| \tilde{\beta}_n - \beta \|_2}{\| \beta \|_2} \right\} \leq 2 \kappa_2^2(X) \frac{(1 + \kappa_2(X) \epsilon) \kappa_2(X)}{1 - \epsilon \kappa_2^2(X)} \frac{\sqrt{m}}{\| \beta \|_2}.$$

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For any $\tau > 1$ the inequality
\[ \frac{\|\tilde{\beta}_N - \beta\|_2}{\|\beta\|_2} \leq \frac{2\kappa_2^2(X)}{1 - \epsilon\kappa_2^2(X)} \epsilon + \frac{(1 + \kappa_2(X)\epsilon)\kappa_2(X)}{1 - \epsilon\kappa_2^2(X)} \frac{\tau \sqrt{m}}{\|X\|_2\|\beta\|_2} \] (27)
holds with probability as least $1 - \exp\left(-\frac{m}{\tau}(\tau - 1)^2\right)$.

Proof. From (11) and (21) we have
\[ X^T X(\tilde{\beta}_N - \beta) = X^T v + \Delta c - \Delta M\beta - \Delta M(\tilde{\beta}_N - \beta). \]
Then,
\[ \tilde{\beta}_N - \beta = X^T v + (X^T X)^{-1}\Delta c - (X^T X)^{-1}\Delta M\beta - (X^T X)^{-1}\Delta M(\tilde{\beta}_N - \beta). \]
Taking the norm and applying (21) and (11), we obtain
\[ \|\tilde{\beta}_N - \beta\|_2 \leq \|X^T v\|_2 + \|(X^T X)^{-1}\|_2(\|\Delta M\|_2\|\beta\|_2 + \|\Delta c\|_2) \]
\[ + \|(X^T X)^{-1}\|_2\|\Delta M\|_2\|\tilde{\beta}_N - \beta\|_2 \]
\[ \leq \|X^T v\|_2 + \|(X^T X)^{-1}\|_2(\epsilon\|X^T X\|_2\|\beta\|_2 + \epsilon\|X\|_2\|y\|_2) \]
\[ + \epsilon\|(X^T X)^{-1}\|_2\|X^T X\|_2\|\tilde{\beta}_N - \beta\|_2 \]
\[ \leq \kappa_2(X) \frac{\|v\|_2}{\|X\|_2} + \epsilon\kappa_2^2(X) \left(2\|\beta\|_2 + \frac{\|v\|_2}{\|X\|_2}\right) + \epsilon\kappa_2^2(X)\|\tilde{\beta}_N - \beta\|_2. \]
Then,
\[ \frac{\|\tilde{\beta}_N - \beta\|_2}{\|\beta\|_2} \leq \frac{2\kappa_2^2(X)}{1 - \epsilon\kappa_2^2(X)} \epsilon + \frac{(1 + \kappa_2(X)\epsilon)\kappa_2(X)}{1 - \epsilon\kappa_2^2(X)} \frac{\sqrt{m}}{\|X\|_2\|\beta\|_2}, \]
leading to (24).

Taking the mean on both sides of (24) and using (21) we obtain (26). By Lemma 2, from (25) we see that (27) holds with probability at least as large as $1 - \exp\left(-\frac{m}{\tau}(\tau - 1)^2\right)$.

The error bounds in (25) and (27) consist of two parts. The first part is caused by computational rounding errors. The second part is essentially caused by the noise in the measurements. In fact, if $\epsilon\kappa_2^2(X) \leq \alpha$ for some constant $\alpha < 1$, then
\[ \kappa_2(X) \leq \frac{(1 + \kappa_2(X)\epsilon)\kappa_2(X)}{1 - \epsilon\kappa_2^2(X)} \leq \frac{2}{1 - \alpha}\kappa_2(X). \]
Note that above lower and upper bounds are independent of $\epsilon$ and their ratio is constant.

In the absence of rounding errors, i.e., $\epsilon = 0$, then $\tilde{\beta}_n = \beta_{ls}$ and it is easy to see that (27) is equivalent to

$$\|\beta_{ls} - \beta\|_2 \leq \sqrt{m} \tau \|X^\dagger\|_2,$$  \hspace{1cm} (28)

which holds with probability as least as large as $1 - \exp\left(-\frac{m}{\tau}(\tau - 1)^2\right)$. This is what we would obtain from $\|\beta_{ls} - \beta\|_2 \leq \|X^\dagger\|_2 \|v\|_2$ and applying Lemma 2. The bound (17) in Theorem 1 indicates that for any $\bar{\tau} > 1$ the inequality

$$\|\beta_{ls} - \beta\|_2 \leq \bar{\tau} \sigma \|X^\dagger\|_2$$  \hspace{1cm} (29)

holds with probability as least as large as $1 - \exp\left(-\frac{1}{\bar{\tau}}(\bar{\tau} - 1)^2\right)$. If we set $\bar{\tau} = 1 + \sqrt{m}(\tau - 1)$, then this probability bound becomes $1 - \exp\left(-\frac{m}{2}(\tau - 1)^2\right)$, while (29) becomes

$$\|\beta_{ls} - \beta\|_2 \leq (\sqrt{m} \tau - \sqrt{m} + 1) \sigma \|X^\dagger\|_2,$$

which is sharper than (28).

In order to obtain a corresponding result when the LS solution is computed by a backward stable algorithm, we first need the following lemma.

**Lemma 3.** Suppose $X \in \mathbb{R}^{m \times n}$ has rank $n$ and $\Delta X \in \mathbb{R}^{m \times n}$ is any matrix satisfying $\|X^\dagger\|_2 \|\Delta X\|_2 < 1$. Then

$$\|(X + \Delta X)^\dagger\|_2 \leq \frac{\|X^\dagger\|_2}{1 - \|X^\dagger\|_2 \|\Delta X\|_2}.$$  \hspace{1cm} (30)

**Proof.** See [5, lemma 20.11]. \hfill \square

**Theorem 4.** Let $\kappa_2(X) = \|X\|_2 \|X^\dagger\|_2$ and suppose $\epsilon \kappa_2(X) < 1$. The relative normwise error between the parameter vector $\beta$ in the linear model (11) and the computed LS solution $\tilde{\beta}_n$ obtained by a backward stable method satisfies

$$\frac{\|\tilde{\beta}_n - \beta\|_2}{\|\beta\|_2} \leq \frac{2\kappa_2(X)}{1 - \epsilon \kappa_2(X)} \epsilon + \frac{(1 + \epsilon)\kappa_2(X)}{1 - \epsilon \kappa_2(X)} \frac{\|v\|_2}{\|X\|_2 \|\beta\|_2}$$  \hspace{1cm} (31)
and
\[
\mathbb{E}\left\{ \frac{\|\tilde{\beta}_n - \beta\|_2}{\|\beta\|_2} \right\} \leq \frac{2\kappa_2(X)}{1 - \epsilon\kappa_2(X)} \epsilon + \frac{(1 + \epsilon)\kappa_2(X)}{1 - \epsilon\kappa_2(X)} \frac{\sqrt{m}}{\|X\|_2\|\beta\|_2} \sigma. \tag{32}
\]

For any \( \tau > 1 \) the inequality
\[
\frac{\|\tilde{\beta}_n - \beta\|_2}{\|\beta\|_2} \leq \frac{2\kappa_2(X)}{1 - \epsilon\kappa_2(X)} \epsilon + \frac{(1 + \epsilon)\kappa_2(X)}{1 - \epsilon\kappa_2(X)} \frac{\tau \sqrt{m}}{\|X\|_2\|\beta\|_2} \sigma. \tag{33}
\]
holds with probability as least \( 1 - \exp\left( - \frac{m}{2} (\tau - 1)^2 \right) \).

Proof. From (I) and (22) we have
\[
\tilde{\beta}_n - \beta = (X + \Delta X)^\dagger (y + \Delta y) - \beta
\]
\[
= (X + \Delta X)^\dagger [(y - X\beta) + (X + \Delta X)\beta - \Delta X\beta + \Delta y] - \beta
\]
\[
= (X + \Delta X)^\dagger (v - \Delta X\beta + \Delta y).
\]

Taking norms and using Lemma 3, (22), and (I), we obtain
\[
\|\beta_{LS} - \beta\|_2 \leq \|(X + \Delta X)^\dagger v\|_2 + \|(X + \Delta X)^\dagger\|_2 (\|\Delta X\|_2\|\beta\|_2 + \|\Delta y\|_2)
\]
\[
\leq \frac{\|X\|_2\|v\|_2}{1 - \epsilon\kappa_2(X)} + \frac{\|X\|_2}{1 - \epsilon\kappa_2(X)} (\epsilon\|X\|_2\|\beta\|_2 + \epsilon\|y\|_2)
\]
\[
\leq \frac{2\kappa_2(X)}{1 - \epsilon\kappa_2(X)} \epsilon + \frac{(1 + \epsilon)\kappa_2(X)}{1 - \epsilon\kappa_2(X)} \frac{\|v\|_2}{\|X\|_2}
\]
leading to (31).

Then from (31), by (23) in Lemma 4 we obtain (32), and by (24) in Lemma 4 we see that (32) holds with probability as least \( 1 - \exp\left( - \frac{m}{2} (\tau - 1)^2 \right) \).

Like those in (22) and (23), the error bounds in (31) and (32) consist of two parts. The first part is caused by computational rounding errors and the second one is essentially caused by the noise in the measurements (see the argument we gave for the error bounds in Theorem 3).

Notice that the bounds in Theorem 4 are smaller than those for the normal equations in Theorem 3. We compare the results of Theorem 4 and Theorem 4 more thoroughly in the following section.
4. Choice of algorithm

A natural question is which of the two, the normal equations method (N) or a backward stable algorithm (B), should be used for linear regression problems. In this section, we attempt to address this question. We consider this question from the point of view of efficiency and accuracy. We suppose that a user wishes to use the most computationally efficient algorithm, as long as this does not sacrifice any accuracy in the computed solution.

When \( m \approx n \), the two algorithms have a similar cost. In this case, B should be used as it provides a more accurate solution than N. When \( m \) is larger than \( n \), N is more efficient than B and can be up to twice as fast as B in terms of flops when \( m \gg n \). If computational efficiency is a concern, and \( \bar{\beta}_N \) is not less accurate than \( \bar{\beta}_B \), one should use N.

General statements similar to the above are made in [15]. In the following we use our results from the previous sections to compare more precisely the accuracy of \( \bar{\beta}_N \) and \( \bar{\beta}_B \) with respect to the parameter vector \( \beta \) in linear regression.

If \( \kappa_2(X) \gtrsim \epsilon^{-1} \), both B and N are likely to fail, or both \( \bar{\beta}_N \) and \( \bar{\beta}_B \) have almost no accurate digits. The least squares problem is too ill-conditioned. In this case, one may want to apply a regularized LS method instead, or redesign the model (11).

If \( \epsilon^{-1/2} \lesssim \kappa_2(X) < \epsilon^{-1} \) and \( \kappa_2(X) \neq \epsilon^{-1} \), N is likely to fail or \( \bar{\beta}_N \) has almost no accurate digits. In this case, B should be used.

Now we assume \( \kappa_2(X) < \epsilon^{-1/2} \) and \( \kappa_2(X) \neq \epsilon^{-1/2} \). In this case, the second terms in the error bounds in (27) and (33) are very close. Comparing the first terms in the two error bounds, we see the former is about \( \kappa_2(X) \) times as large as the latter. If in the error bound in (27) the second term dominates, i.e.,

\[
\sigma \geq \frac{\|X\|_2 \|\beta\|_2 \kappa_2(X) \epsilon}{\sqrt{m}},
\]

then in the error bound in (33) the second term also dominates. In this case, N should be used, as we expect no significant difference between the two algorithms.
in terms of accuracy of the computed estimates. If (34) does not hold exactly or approximately, B should be used in order to obtain a more accurate computed estimate of β.

As with (18), the difficulty in checking the inequality (34) is that β is unknown. One way to overcome this difficulty is to replace ∥β∥ by an approximation. Note that

\[ \|\beta\|^2 \geq \frac{\|X\beta\|^2}{\|X\|^2} = \frac{\|y - v\|^2}{\|X\|^2} \leq \frac{\|y\|^2 + \|v\|^2}{\|X\|^2} \approx \frac{\|y\|^2 + \sigma \sqrt{m}}{\|X\|^2}. \]  

(35)

where y is a given sample of the random variable y, see (11) and Lemma 4. Substituting ∥β∥ by the most right-hand side in (35) and rearranging, we obtain the criterion

\[ \sigma \geq \frac{\|y\|^2 \kappa_2(X) \epsilon}{\sqrt{m}(1 - \kappa_2(X) \epsilon)}. \]  

(36)

We compare the criteria (34) and (36) in the following section.

5. Numerical examples

In this section we give some numerical examples to illustrate our bounds from Theorem 3 and Theorem 4. Our numerical tests were performed with MATLAB.

In these tests, the matrix X ∈ ℝ^{200×50} is created according to its SVD (7), where U_1 and V are taken to be the “compacted” Q-factors from the QR factorizations of the two random matrices randn(200, 50) and randn(50, 50), respectively, and \( \sigma_1 = 10^{-p+(n-i)\times(1+p)/(n-1)} \) so \( \kappa_2(X) = 10^{p+1} \). We vary p to obtain matrices X having condition numbers \( 10^1, 10^3, 10^5, \ldots, 10^{11} \).

For each matrix X created as described above, we set the parameter vector \( \beta = [\cos(1), \ldots, \cos(n)]^T \). We then pick 20 different values of the noise level \( \sigma \) ranging between \( 10^{-20} \) and 1. For each value of \( \sigma \), we form 1000 different samples \( y \) of y according to (11). For each of these samples, we then compute realizations of the LS solution \( \widehat{\beta}_N \) using the normal equations method and \( \widehat{\beta}_B \) using the backward stable Householder QR factorization method. We then compute the average, over the 1000 different samples, of the normwise relative
Figure 1: Error between the parameter vector and the computed LS solutions versus $\sigma$.

errors $\|\tilde{\beta}_N - \beta\|_2 / \|\beta\|_2$ and $\|\tilde{\beta}_B - \beta\|_2 / \|\beta\|_2$, as well as the respective probabilistic bounds given in (27) and (33) with $\tau = 1.1$. These averages are plotted versus $\sigma$ in Figure 1. For $\kappa_2(X) = 10^9$ and $\kappa_2(X) = 10^{11}$ (see the two bottom plots in Figure 1), only values corresponding to QR are plotted because, for these more ill-conditioned problems with $\kappa_2(X) > \epsilon^{-1/2}$, the Cholesky factorization used in the normal equations method fails and the error estimate (24) for the normal
equations method is not defined.

For these tests, given that $m = 200$ and $\tau = 1.1$, Theorem 3 and Theorem 4 guarantee that the upper bounds hold with probability at least 0.63. In fact, the bounds always held in all of our tests. For both methods, the error bounds are descriptive of the actual error, being only one or two orders of magnitude larger than the actual error.

The solid vertical line in the top four plots in Figure 1 corresponds to the value of $\sigma$ at which equality holds in (34). As predicted in Section 4, when $\sigma$ is smaller than this value (to the left of the vertical line) the backward stable algorithm more accurately recovers the parameter vector $\beta$ than the normal equations, and when $\sigma$ is larger than this value (to the right of the vertical line) both algorithms have more or less the same error, mainly caused by the noise in the model.

In practice, one would use the criterion (36) instead of (34). This criterion depends on the sample $y$. In dotted vertical lines, we plot the minimum and maximum value of $\sigma$, over all 20000 of our tests, at which equality holds in (36). The value of $\sigma$ predicted by (36) is only slightly smaller than that predicted by (34). This shows that the criterion (36) is robust and useful in practice for determining whether the normal equations can safely be used in linear regression problems.

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