

## COMPUTING PROJECTIONS WITH LSQR\*

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**Abstract.**

LSQR uses the Golub-Kahan bidiagonalization process to solve sparse least-squares problems with and without regularization. In some cases, projections of the right-hand side vector are required, rather than the least-squares solution itself. We show that projections may be obtained from the bidiagonalization as linear combinations of (theoretically) orthogonal vectors. Even the least-squares solution may be obtained from orthogonal vectors, perhaps more accurately than the usual LSQR solution. (However, LSQR has proved equally good in all examples so far.)

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**1 Introduction.**

LSQR [11, 12] is a conjugate-gradient-like method for solving linear least-squares problems

$$(1.1) \quad \min_x \|b - Ax\|_2,$$

where  $A$  is a real  $m \times n$  matrix and  $b$  is a real vector. Typically  $m \geq n$  and  $\text{rank}(A) = n$ , though not necessarily. LSQR uses the Golub-Kahan bidiagonalization of  $A$  [6] with starting vector  $b$ , forming a sequence of iterates  $\{x_k\}$  to approximate  $x$ .

For problem (1.1), let us define the following items:

$$(1.2) \quad P = A(A^T A)^{-1} A^T,$$

$$(1.3) \quad x = (A^T A)^{-1} A^T b,$$

$$(1.4) \quad p = Pb = Ax,$$

$$(1.5) \quad r = (I - P)b = b - Ax,$$

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where  $P$  and  $(I - P)$  are both projection operators. Since some applications need  $p$  or  $r$  rather than  $x$  itself, and since these projections are less sensitive than  $x$  to perturbations in the data [7], it seems reasonable to compute the projections directly from the Golub-Kahan process, rather than from LSQR's final approximation to  $x$ .

Section 3.1 shows how to compute  $p$  and  $r$  for problem (1.1). Section 4.1 does the same for regularized or *damped* least-squares problems, and suggests some unexpected new ways for computing  $x$ .

### 1.1 Orthogonal steps.

If a sequence of approximations  $\{x_k\}$  is computed in the form

$$(1.6) \quad x_k = V_k y_k = x_{k-1} + \eta_k v_k,$$

where the columns of  $V_k$  are (at least theoretically) orthonormal ( $V_k^T V_k = I$ ), we say that  $x$  is computed by *orthogonal steps*. For example, Craig's method [4, 5, 11] solves unsymmetric equations  $Ax = b$  using orthogonal steps (1.6) to update each  $x_k$ . In contrast, the normal LSQR iterates have the form

$$(1.7) \quad x_k = (V_k R_k^{-1}) z_k \equiv W_k z_k = x_{k-1} + \zeta_k w_k,$$

where  $V_k$  is orthonormal but  $W_k$  is not. If the triangular matrix  $R_k$  is ill-conditioned, we would expect a certain loss of precision (via cancellation) in forming  $x_k$  that way.

A contribution of this paper is to show that for least-squares problems with and without damping,  $x$ ,  $p$  and  $r$  can all be computed by orthogonal steps.

## 2 Bidiagonalization.

Given a general matrix  $A$  and a starting vector  $b$ , the Golub-Kahan process generates two sequences of vectors  $\{u_k\}$ ,  $\{v_k\}$  and positive scalars  $\{\alpha_k\}$ ,  $\{\beta_k\}$  such that after  $k$  steps,

$$(2.1) \quad \begin{aligned} AV_k &= U_{k+1} B_k, \\ A^T U_{k+1} &= V_k B_k^T + \alpha_{k+1} v_{k+1} e_{k+1}^T, \\ U_k &= (u_1 \ u_2 \ \dots \ u_k), \\ V_k &= (v_1 \ v_2 \ \dots \ v_k), \end{aligned} \quad B_k = \begin{pmatrix} \alpha_1 & & & \\ \beta_2 & \ddots & & \\ & \ddots & \alpha_k & \\ & & & \beta_{k+1} \end{pmatrix},$$

where  $B_k$  is  $(k+1) \times k$  and lower bidiagonal. The starting condition is  $\beta_1 u_1 = b$ , so that  $U_k \beta_1 e_1 = b$  exactly for all  $k$ , and with exact arithmetic the columns of  $U_k$  and  $V_k$  would be orthonormal.

## 3 Least squares.

To solve problem (1.1), LSQR defines a sequence of approximations  $x_k = V_k y_k$ , where each  $y_k$  is defined by a subproblem,  $\min \|\beta_1 e_1 - B_k y_k\|$  [11, 13]. The

subproblem is reliably solved via a QR factorization of  $B_k$ :

$$Q_k(B_k \beta_1 e_1) = \begin{pmatrix} R_k & z_k \\ & \bar{\zeta}_k \end{pmatrix}, \quad R_k y_k = z_k,$$

where  $R_k$  is  $k \times k$  and upper bidiagonal. The matrix  $Q_k$  is nominally a product of  $k$  plane rotations, requiring little work. In LSQR we work with symmetric transformations for simplicity. The  $k$ th transformation is of the form

$$\begin{pmatrix} c_k & s_k \\ s_k & -c_k \end{pmatrix} \begin{pmatrix} \bar{\rho}_{k-1} & 0 & \bar{\zeta}_{k-1} \\ \beta_{k+1} & \alpha_{k+1} & 0 \end{pmatrix} = \begin{pmatrix} \rho_k & \theta_k & \zeta_k \\ & \bar{\rho}_k & \bar{\zeta}_k \end{pmatrix},$$

where  $\bar{\zeta}_k$  later becomes  $\zeta_{k+1}$  (and similarly for other barred items). To keep storage to a minimum,  $y_k$  is eliminated and  $x_k$  is formed as in (1.7).

### 3.1 Projections.

As approximations to the projections  $p = Pb$  and  $r = (I - P)b$ , we use the vectors  $p_k = Ax_k$  and  $r_k = b - Ax_k$ . Let us write the (theoretically orthonormal) matrix  $U_{k+1}Q_k^T$  as

$$(3.1) \quad U_{k+1}Q_k^T = (U1_k \bar{u}_k),$$

in which the  $k$ th transformation has the form

$$(\bar{u}_{k-1} \ u_{k+1}) \begin{pmatrix} c_k & s_k \\ s_k & -c_k \end{pmatrix} = (u1_k \ \bar{u}_k).$$

It follows that

$$\begin{aligned} p_k &= Ax_k = AV_k y_k = U_{k+1} B_k y_k \\ &= U_{k+1} Q_k^T Q_k B_k y_k \\ &= (U1_k \ \bar{u}_k) \begin{pmatrix} R_k \\ 0 \end{pmatrix} y_k \\ &= (U1_k \ \bar{u}_k) \begin{pmatrix} z_k \\ 0 \end{pmatrix} = U1_k z_k \end{aligned}$$

and

$$\begin{aligned} r_k &= b - Ax_k \\ &= U_{k+1} Q_k^T Q_k (\beta_1 e_1 - B_k y_k) \\ &= (U1_k \ \bar{u}_k) \left\{ \begin{pmatrix} z_k \\ \bar{\zeta}_k \end{pmatrix} - \begin{pmatrix} R_k \\ 0 \end{pmatrix} y_k \right\} \\ &= (U1_k \ \bar{u}_k) \begin{pmatrix} 0 \\ \bar{\zeta}_k \end{pmatrix} = \bar{\zeta}_k \bar{u}_k. \end{aligned}$$

Thus, the sequences  $\{p_k\}$  and  $\{r_k\}$  are obtained by orthogonal steps. The main expense beyond the bidiagonalization lies in forming the columns of  $U1_k$  in (3.1). Note that  $x_k$  need not be formed.

**4 Damped least squares.**

The damped least-squares problem is

$$(4.1) \quad \min \|b - Ax\|^2 + \|\delta x\|^2 \equiv \min \left\| \begin{pmatrix} b \\ 0 \end{pmatrix} - \begin{pmatrix} A \\ \delta I \end{pmatrix} x \right\|^2,$$

where  $\delta > 0$  is a small scalar that regularizes the problem if  $\text{rank}(A) < n$  or  $A$  is ill-conditioned. For such problems, LSQR uses the same bidiagonalization to obtain approximations  $x_k = V_k y_k$ , where  $y_k$  is defined by the subproblem

$$\min \left\| \begin{pmatrix} \beta_1 e_1 \\ 0 \end{pmatrix} - \begin{pmatrix} B_k \\ \delta I \end{pmatrix} y_k \right\|,$$

which is solved via an extended QR factorization [2, 12, 13]:

$$Q_k \begin{pmatrix} B_k & \beta_1 e_1 \\ \delta I & 0 \end{pmatrix} = \begin{pmatrix} R_k & z_k \\ & \bar{\zeta}_k \\ & q_k \end{pmatrix}, \quad R_k y_k = z_k.$$

The matrix  $Q_k$  now involves a product of  $2k$  transformations, but the total work and storage is essentially the same as when  $\delta = 0$ . As before,  $y_k$  is eliminated and  $x_k$  is formed as in (1.7).

*4.1 Projections.*

The damped least-squares solution satisfies  $(A^T A + \delta^2 I)x = A^T b$ . With

$$\bar{A} = \begin{pmatrix} A \\ \delta I \end{pmatrix}, \quad \bar{b} = \begin{pmatrix} b \\ 0 \end{pmatrix},$$

the definitions analogous to (1.2)–(1.5) are

$$(4.2) \quad \bar{P} = \bar{A}(\bar{A}^T \bar{A})^{-1} \bar{A}^T,$$

$$(4.3) \quad x = (\bar{A}^T \bar{A})^{-1} \bar{A}^T \bar{b},$$

$$(4.4) \quad \begin{pmatrix} p \\ s \end{pmatrix} = \bar{P} \bar{b} = \begin{pmatrix} Ax \\ \delta x \end{pmatrix},$$

$$(4.5) \quad \begin{pmatrix} r \\ t \end{pmatrix} = (I - \bar{P}) \bar{b} = \begin{pmatrix} b - Ax \\ -\delta x \end{pmatrix},$$

where we see that  $s = -t = \delta x$ . Now define the (theoretically orthonormal) matrix

$$(4.6) \quad \begin{pmatrix} U_{k+1} & \\ & V_k \end{pmatrix} Q_k^T = \begin{pmatrix} U1_k & \bar{u}_k & U2_k \\ V1_k & \bar{v}_k & V2_k \end{pmatrix},$$

where the next two transformations defining  $Q_{k+1}$  leave  $U1_k$ ,  $U2_k$ ,  $V1_k$ ,  $V2_k$  unaltered. It follows that

$$\begin{aligned} \begin{pmatrix} p_k \\ \delta x_k \end{pmatrix} &= \begin{pmatrix} Ax_k \\ \delta x_k \end{pmatrix} = \begin{pmatrix} AV_k \\ \delta V_k \end{pmatrix} y_k = \begin{pmatrix} U_{k+1} B_k \\ \delta V_k \end{pmatrix} y_k \\ &= \begin{pmatrix} U_{k+1} & \\ & V_k \end{pmatrix} Q_k^T Q_k \begin{pmatrix} B_k \\ \delta I \end{pmatrix} y_k \\ &= \begin{pmatrix} U1_k & \bar{u}_k & U2_k \\ V1_k & \bar{v}_k & V2_k \end{pmatrix} \begin{pmatrix} z_k \\ 0 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} U1_k z_k \\ V1_k z_k \end{pmatrix}, \end{aligned}$$

and

$$\begin{aligned} \begin{pmatrix} r_k \\ -\delta x_k \end{pmatrix} &= \begin{pmatrix} b \\ 0 \end{pmatrix} - \begin{pmatrix} Ax_k \\ \delta x_k \end{pmatrix} \\ &= \begin{pmatrix} U_{k+1} & \\ & V_k \end{pmatrix} Q_k^T Q_k \left\{ \begin{pmatrix} \beta_1 e_1 \\ 0 \end{pmatrix} - \begin{pmatrix} B_k \\ \delta I \end{pmatrix} y_k \right\} \\ &= \begin{pmatrix} U1_k & \bar{u}_k & U2_k \\ V1_k & \bar{v}_k & V2_k \end{pmatrix} \left\{ \begin{pmatrix} z_k \\ \bar{\zeta}_k \\ q_k \end{pmatrix} - \begin{pmatrix} R_k \\ 0 \\ 0 \end{pmatrix} y_k \right\} \\ &= \begin{pmatrix} \bar{u}_k & U2_k \\ \bar{v}_k & V2_k \end{pmatrix} \begin{pmatrix} \bar{\zeta}_k \\ q_k \end{pmatrix}. \end{aligned}$$

Thus, the sequences  $\{p_k\}$ ,  $\{r_k\}$  and  $\{\delta x_k\}$  are obtained by orthogonal steps:

$$(4.7) \quad p_k = U1_k z_k,$$

$$(4.8) \quad r_k = U2_k q_k + \bar{\zeta}_k \bar{u}_k,$$

$$(4.9) \quad \delta x_k = V1_k z_k,$$

$$(4.10) \quad -\delta x_k = V2_k q_k + \bar{\zeta}_k \bar{v}_k.$$

We see that the ‘‘damped’’ projections have led to two new sequences for approximating  $x$ . We shall denote these by  $\{x1_k\}$  and  $\{x2_k\}$ . To use (4.7)–(4.10) in the usual way, we form

$$(4.11) \quad p_k = p_{k-1} + \zeta_k u1_k,$$

$$(4.12) \quad \hat{r}_k = \hat{r}_{k-1} + \psi_k u2_k,$$

$$(4.13) \quad \hat{x}1_k = \hat{x}1_{k-1} + \zeta_k v1_k,$$

$$(4.14) \quad \hat{x}2_k = \hat{x}2_{k-1} + \psi_k v2_k,$$

and upon termination at step  $k$  we make some final adjustments:

$$(4.15) \quad r_k = \hat{r}_k + \bar{\zeta}_k \bar{u}_k,$$

$$(4.16) \quad x1_k = (1/\delta)\hat{x}1_k,$$

$$(4.17) \quad x2_k = -(1/\delta)(\hat{x}2_k + \bar{\zeta}_k \bar{v}_k).$$

#### 4.2 Discussion.

1. The approximations  $x_k$ ,  $p_k$  and  $r_k$  are defined for all  $\delta \geq 0$ , but  $x1_k$  and  $x2_k$  require  $\delta > 0$ .
2. In (4.16)–(4.17), the divisions by  $\delta$  may appear hazardous as  $\delta \rightarrow 0$ . However, the norm of each column of  $V1_k$  and  $V2_k$  is of order  $\delta$ , and  $\|z_k\|$ ,  $\|q_k\|$  and  $|\bar{\zeta}_k|$  are all bounded by  $\|b\|$ . Values as small as  $\delta = 10^{-10}$  (say) seem to be safe in practice. Hence,  $x1_k$  or  $x2_k$  may be used to estimate  $x$  for both normal and damped least squares.
3. The Golub-Kahan process requires work vectors  $u$  and  $v$  ( $m + n$  storage locations) and  $3m + 3n$  floating-point operations (flops) per step, as well as the usual products  $u \leftarrow Av + u$ ,  $v \leftarrow A^T u + v$ .
4. Table 4.1 shows the additional storage and work needed to estimate various vectors. For example, to estimate  $x$ , LSQR uses work vectors  $x$  and  $w$  ( $2n$  storage locations) and  $2n$  flops per step, for all values of  $\delta$ . The other quantities are somewhat more expensive.
5. To implement reliable stopping rules, LSQR uses the vectors  $w_k$  to estimate  $\text{cond}(\bar{A})$ . When  $x$  is being estimated, this involves no additional storage and  $2n$  additional flops per step. If  $p$ ,  $r$ ,  $x1$  or  $x2$  are estimated but not  $x$ , the extra cost to estimate  $\text{cond}(\bar{A})$  is  $n$  locations and  $3n$  flops per step.
6.  $x1$  is slightly cheaper to compute than  $x2$ , and to date the computational results have not favored one over the other. It is probably sufficient to consider  $x1$ .

In summary, computing all of  $p$ ,  $r$  and  $x1$  requires about twice the storage and work compared to the usual LSQR  $x$ . This may not be significant if the matrix-vector products dominate.

## 5 Relationship to Craig's method.

Craig's method [4, 5] solves *compatible* rectangular systems of the form

$$(5.1) \quad \min \|x\| \quad \text{subject to} \quad Ax = b,$$

where we typically have  $m \leq n$  and  $\text{rank}(A) = m$ . As described in [10, 11], the method may be implemented via  $\text{Bidiag}(A, b)$ , the Golub-Kahan bidiagonalization of  $A$  with starting vector  $b$ . This seems to be a reliable approach, but an outstanding question has been: What if the right-hand side is of the

Table 4.1: Storage and work per step needed (excluding the bidiagonalization) to estimate the normal LSQR solution  $x$ , the projections  $p$  and  $r$ , and the new solution estimates  $x1$  and  $x2$ .

	Vectors	Storage	Work	
			$\delta = 0$	$\delta > 0$
$x$	$x, w$	$2n$	$2n$	$2n$
$p$	$p, \bar{u}$	$2m$	$3m$	$5m$
$r$	$r, \bar{u}$	$2m$	$2m$	$4m$
$p$ and $r$	$p, r, \bar{u}$	$3m$	$4m$	$6m$
$x1$	$x1, \bar{v}$	$2n$		$4n$
$x2$	$x2, \bar{v}$	$2n$		$5n$

form  $b = Ac$ ? The method is then using  $\text{Bidiag}(A^T, Ac)$ , which is *not* a reliable approach [11, 3].

This curiosity is now resolved by noting that when  $b = Ac$ , the solution to (5.1) is  $x = A(AA^T)^{-1}Ac$ , which is the projection  $p = Pc$  associated with the least-squares problem  $\min_y \|c - A^T y\|$ . The method of Section 3 may be applied. Similarly, minimum-length problems of the form

$$(5.2) \quad \min \|x\|^2 + \|s\|^2 \quad \text{subject to} \quad Ax + \delta s = b,$$

may be treated by LSQR or by an extension of Craig's method as described in [13], but if  $b = Ac$ , then the method of Section 4 may be applied to compute  $(x, s)$  as a projection.

## 6 Computational results.

The test problems described in [11] were generalized slightly to include damping and arbitrary values of  $m$  and  $n$ . They use a matrix of the form  $A = YDZ$ , where  $Y$  and  $Z$  are Householder transformations and  $D$  is diagonal with prescribed singular values. Preliminary conclusions follow.

Note that when  $m = n$  and  $\delta = 0$ , the exact projections are  $p = b$  and  $r = 0$ . Also, when  $\delta = 0$ ,  $x1$  and  $x2$  are undefined. These cases were not considered.

For the results obtained, the machine precision was  $\epsilon \approx 10^{-16}$ ; the damping parameter was in the range  $10^{-11} \leq \delta \leq 10^{-8}$ ;  $\|A\|$ ,  $\|b\|$  and  $\|x\|$  were all  $O(1)$ ; and the condition of the "damped" matrix was in the range  $10^6 \leq \text{cond}(\bar{A}) \leq 10^{11}$ . The stopping tolerances for LSQR were  $\text{atol} = \text{btol} = \epsilon^{0.9} \approx 10^{-14}$ .

Below,  $p$ ,  $r$ ,  $x$ ,  $x1$  and  $x2$  mean the final computed estimates of  $p$ ,  $r$  and  $x$ .

### 6.1 Observations.

1. When  $m = n$  and  $\|r\| = O(\epsilon)$ , the errors in  $p$  and  $r$  were  $O(\text{atol})$ , and the errors in  $x$ ,  $x1$  and  $x2$  grew in proportion to  $\text{cond}(\bar{A})$ . This matches the sensitivity of the problem itself, indicating stability [7].

2. When  $m > n$  or  $m < n$  and  $\|r\| = O(10^{-6})$ , the same results were observed.
3. When  $m > n$  and  $\|r\| > 10^{-3}$ , the errors in  $x$ ,  $x1$  and  $x2$  grew in proportion to  $\text{cond}(\bar{A})^2$ . Again this matches the sensitivity of least-squares problems.
4. In the same cases ( $\|r\|$  large), the errors in  $p$  and  $r$  grew with  $\text{cond}(\bar{A})$  in accordance with sensitivity analysis, but they were significantly smaller than could be expected from the actual size of  $\text{cond}(\bar{A})$ .
5. The final  $p$  and  $r$  closely matched  $Ax$  and  $b - Ax$  computed from the final LSQR estimate of  $x$ .
6. Surprisingly, this was true even when  $x$  had essentially no digits of precision.
7. More surprisingly, the three estimates  $x$ ,  $x1$  and  $x2$  matched each other very closely in all cases, even when they all had no correct digits. In extreme cases,  $x$  and  $x1$  agreed more closely than  $x$  and  $x2$ .

Support for Observations 4 and 5 has been given by Björck *et al.* [1, 3], who study the “recursive residuals” for various CG methods including CGLS, the original least-squares algorithm of Hestenes and Stiefel [9]. For updates such as (1.7), the recursive residuals are defined by

$$(6.1) \quad \begin{aligned} x_k &= x_{k-1} + \zeta_k w_k, \\ \tilde{r}_k &= \tilde{r}_{k-1} - \zeta_k A w_k, \end{aligned}$$

where we use  $\tilde{r}_k$  to distinguish from  $r_k$  in Sections 3–4. In CGLS the residuals are an integral part of the iteration. In LSQR they are not normally needed, but they may be computed for interest.

Following Greenbaum [8], Björck *et al.* [3] prove for CGLS and LSQR that  $\tilde{r}_k$  closely approximates  $b - Ax_k$  for all  $k$ . This matches Observation 5.

They also conjecture from experimental evidence that  $\tilde{r}_k$  is ultimately very close to the true residual  $r$ . This is confirmed by Observation 4; for example, with  $\text{cond}(\bar{A}) = 10^{11}$  and  $\|r\| = 10$ , the final value of  $\|r - \tilde{r}_k\|/\|r\|$  was  $10^{-9}$  rather than the expected  $10^{-5}$ .

## 7 Conclusions.

We have shown how to obtain projections  $p = Ax$  and  $r = b - Ax$  from the Golub-Kahan process, as well as two different estimates of  $x$ , using orthogonal steps for all quantities. We were motivated by the concern that updates of the form (6.1) could entail significant cancellation if both  $\zeta_k$  and  $\|w_k\|$  are large.

In LSQR, we know that some of the vectors  $w_k$  can be large, because  $\|W_k\|$  is used to estimate  $\text{cond}(A)$ . However, for the present test problems the corresponding multipliers  $\zeta_k$  were always small (see [13]). Thus, we have not yet seen a benefit from obtaining  $p$ ,  $r$ ,  $x1$  and  $x2$  by orthogonal steps.



Since the new approach for computing projections involves additional work and storage, it is probably best to compute  $x$  via the standard CGLS or LSQR iterations and then form  $p$  or  $r$  directly. We recommend this even in ill-conditioned cases where the computed  $x$  has no accuracy. If cases arise in which the errors in  $p$ ,  $r$  or  $x$  exceed whatever can be expected from  $\text{cond}(A)$ , the methods of this paper should be reconsidered.

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