Mathematics in Signal Processing.
T. S. Durrani, J. B. Abbiss, J. E. Hudson, R. N. Madan, J. G. McWhirter, and T. A. Moore (editors).
Oxford University Press, 1987.

# THE NUMERICAL SOLUTION OF THE GENERAL GAUSS-MARKOV LINEAR MODEL.

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#### INTRODUCTION

In this contribution we give an overview of the numerical solution of the general Gauss-Markov linear model given by

$$y = X\beta + e$$
,  $e \subseteq N(O, \sigma^2 W)$ , (1.1)

where the notation  $eCN(0,\sigma^2W)$  indicates that the noise vector e is assumed to come from a normal distribution with mean zero and variance-covariance matrix  $\sigma^2W$ , W being a symmetric nonnegative definite matrix.

We start by considering the standard case where W=I, then consider the more general case where W is any non-singular positive definite matrix and finally we consider the case where W is allowed to be singular. The material in this contribution is not new, but deserves an airing since it provides us with the basic tools for the reliable implementation of least-squares problems and the Kalman filter, and on a variety of architectures.

# 2. THE STANDARD GAUSS-MARKOV LINEAR MODEL

In this section we look at the standard model

$$y = X\beta + e$$
,  $eCN(O, \sigma^2I)$ . (2.1)

The associated linear least-squares problem for this model is given by

$$\min \hat{e}^{T} \hat{e}, \quad \hat{e} = \hat{y} - \hat{x}b, \qquad (2.2)$$

where  $\hat{X}$  is the n by p matrix of observations,  $\hat{y}$  the n element vector of dependent observations, b is the p element vector of regression coefficients and  $\hat{e}$  is the n element error vector. Throughout this article we shall assume that there are at least as many observations as variables so that  $n \geqslant p$ , although much of the discussion is readily extended to the underdetermined case.

Tools for the reliable solution of (2.2) are the QR factorization and the singular value decomposition (SVD). In the next section we describe these factorizations. We shall not give the algorithmic detail of computing these factorizations, but instead give appropriate references.

## 3. THE OR FACTORIZATION AND THE SVD

The QR factorization of an n by p matrix X is given by

$$X = Q \begin{bmatrix} R \\ O \end{bmatrix} , \qquad (3.1)$$

where Q is an n by n orthogonal matrix and R is a p by p upper triangular matrix. The SVD of X is given by

$$X = U \left[ D \right] V^{T}, \tag{3.2}$$

where U is an n by n orthogonal matrix, V is a p by p orthogonal matrix and D is a diagonal matrix with non-negative diagonal elements called the  $\underline{\text{singular values}}$  of X. The factorization can be chosen so that the singular values are in descending order down D. The first p columns of U are the left singular vectors of X and the columns of V are the right singular vectors of X.

If we perform the QR factorization (3.1) and then perform an SVD of R as  $\,$ 

$$R = \hat{\mathbf{U}}\hat{\mathbf{D}}\hat{\mathbf{V}}^{\mathrm{T}} \tag{3.3}$$

then

$$x = Q \begin{bmatrix} \widetilde{U}D\widetilde{V}^{T} \\ O \end{bmatrix} = Q \begin{bmatrix} \widetilde{U} & O \\ O & I \end{bmatrix} \begin{bmatrix} \widetilde{D} \\ O \end{bmatrix} \quad \widetilde{V}^{T}$$

$$= U \begin{bmatrix} D \\ C \end{bmatrix} \quad V^{T}, \quad U = Q \begin{bmatrix} \widetilde{U} & O \\ O & I \end{bmatrix}, \quad D = \widetilde{D}, \quad V = \widetilde{V}$$
 (3.4)

and hence X and R have the same singular values and right singular vectors.

From (3.1) and (3.2) we find that

$$x^{T}x = R^{T}R$$

$$= VD^{2}V^{T},$$
(3.5)

which are respectively the Cholesky and spectral factorizations of  $x^Tx$ . Thus R and (V,D) give us alternative compact representations of  $x^Tx$  without having to take the numerically damaging step of explicitly forming  $x^Tx$ . (Golub, 1965; Hammarling, 1985.)

For many applications we can use the QR factorization when X is not close to being rank deficient, but carry on to the SVD otherwise. The SVD is a powerful tool for the analysis of rank deficient and near rank deficient problems. For example, from (3.2)

$$xv_j = d_j u_j$$

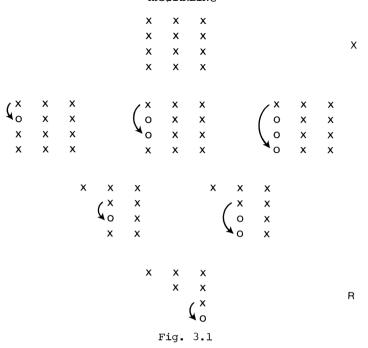
where  $d_j$ ,  $u_j$  and  $v_j$  are respectively the jth singular value, left singular vector and right singular vector of X. Thus

$$||\mathbf{x}\mathbf{v}_{\mathbf{j}}||_2 = \mathbf{d}_{\mathbf{j}}$$

so that right singular vectors that correspond to small singular values give information on the near linear dependencies in the columns of  $X_{\bullet}$ 

Both the QR factorization and the SVD can be obtained by numerically stable methods, based upon orthogonal transformations, and there are a number of sources of quality software that implement these methods. For background on both factorizations, the algorithms to compute them and many further references see Golub and Van Loan (1983).

For signal processing applications, a useful transformation is the plane rotation. This transformation is flexible and, unlike the hyperbolic rotation, is orthogonal and therefore has the desired numerical stability. Plane rotations are described in the above reference and in Figure 3.1 we illustrate the progress from X to R using the standard sequence of plane rotations for the case n=4, p=3. (Givens, 1958.)



A number of other sequences are possible, based upon introducing zeros into a column in different orders and two such alternative orderings are illustrated in Figure 3.2.



Fig. 3.2

Similarly we can perform plane rotations in disjoint planes in parallel, an idea that originates from a paper on error analysis for the QR factorization! (Gentleman, 1975; see also Modi and Clarke, 1984.) One such sequence for the case n=8, p=6 is illustrated in Figure 3.3, where rotations with the same index can be performed in parallel.

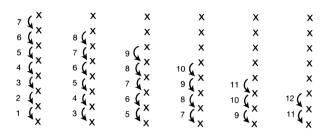


Fig. 3.3

The number of parallel operations for the illustrated sequence is (n+p-2) as opposed to  $\frac{1}{2}p(2n-p-1)$  serial operations.

We can also readily update an existing QR factorization with additional observations as they become available, a particularly important feature for real time computing. This is illustrated in Figure 3.4 for the case p=3.

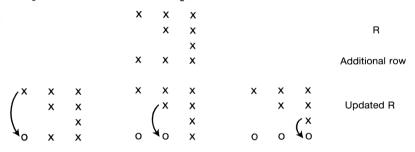


Fig. 3.4

These ideas form the basis of the systolic array implementation of the QR factorization. (Gentleman and Kung, 1981.)

For the SVD, as already mentioned, we can first apply the QR factorization and then find the SVD of R. The classical method of computing the SVD is to use the method originating with Golub and Kahan (1965) and realized as an Algol 60 algorithm by Golub and Reinsch (1970), in which R is reduced to bi-diagonal form and then the implicit QR algorithm is used to further reduce this to diagonal form. We note that R may be reduced to bi-diagonal form by applying plane rotations from both sides. This computation of the SVD is illustrated in Figure 3.5. The method corresponds to the reduction of

 $\boldsymbol{R}^{\mathrm{T}}\boldsymbol{R}$  to tri-diagonal form, followed by the QR algorithm applied to the tri-diagonal form.

Fig. 3.5

More recently a method due to Kogbetliantz (1955) has been revived and in this method R is iteratively reduced to diagonal form, corresponding to Jacobi's method applied to  $R^TR$ . In Jacobi's method each plane rotation is chosen to solve the two by two symmetric eigenvalue problem so that  $c=\cos\theta$  and  $s=\sin\theta$  are such that

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x & y \\ y & z \end{bmatrix} \begin{bmatrix} c & -s \\ s & c \end{bmatrix} = \begin{bmatrix} x' & 0 \\ 0 & z' \end{bmatrix}$$

and a sweep of Jacobi's method applies  $\frac{1}{2}n(n-1)$  such transformations with

$$\begin{bmatrix} x & y \\ y & z \end{bmatrix} = \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{bmatrix}$$

for each i and j (j>l). The usual method chooses i and j cyclically, but other orderings are possible and, as with the QR algorithm we can apply transformations in parallel. (Modi, 1982; Modi and Parkinson, 1982.)

In the Kogbetliantz method (Figure 3.6) each transformation solves the two by two SVD problem, so that the left and right rotations are such that

$$\begin{bmatrix} c_1 & s_1 \\ -s_1 & c_1 \end{bmatrix} \begin{bmatrix} x & y \\ y' & z \end{bmatrix} \begin{bmatrix} c_2 & -s_2 \\ s_2 & c_2 \end{bmatrix} = \begin{bmatrix} x' & 0 \\ 0 & z' \end{bmatrix}$$

and one sweep of the method corresponds to one sweep of Jacobi. In the cyclic ordering one sweep makes R lower triangular and a second sweep restores the upper triangle. The Kogbetliantz approach is the basis of a systolic array

implementation of the SVD. (Brent and Luk, 1985.)

Fig. 3.6

# 4. SOLVING THE STANDARD LINEAR LEAST-SQUARES PROBLEM

In this section we consider the solution of the least-squares problem  $\ \ \,$ 

$$\min \hat{e}^{T} \hat{e}, \quad \hat{e} = \hat{y} - \hat{x} b \tag{4.1}$$

using the QR factorization of (3.1) and the SVD. If we put

$$\varrho^{T}\hat{\mathbf{e}} = \mathbf{f} \equiv
\begin{bmatrix}
\mathbf{f}_{1} \\
\mathbf{f}_{2}
\end{bmatrix}, \quad \varrho^{T}\hat{\mathbf{y}} = \mathbf{z} \equiv
\begin{bmatrix}
\mathbf{z}_{1} \\
\mathbf{z}_{2}
\end{bmatrix}$$

then, since  $f^T f = \hat{e}^T \hat{e}$ , (4.1) becomes

min 
$$f^T f$$
,  $f = z - \begin{bmatrix} z \\ 0 \end{bmatrix} b = \begin{bmatrix} z_1 - Rb \\ z_2 \end{bmatrix}$  (4.2)

If  $\hat{X}$  has full rank so that R is non-singular, we can choose b as the solution of the upper triangular equations

$$Rb = z_1 \tag{4.3}$$

and hence this solves (4.2). Thus

$$\hat{\mathbf{e}}^{\mathrm{T}}\hat{\mathbf{e}} = \mathbf{z}_{2}^{\mathrm{T}}\mathbf{z}_{2}.\tag{4.4}$$

If  $\hat{X}$  does not have full rank we can proceed with the SVD of R

$$R = \mathbf{\hat{U}} \mathbf{D} \mathbf{V}^{\mathrm{T}} \tag{4.5}$$

and (4.2) is equivalent to

min 
$$f_1^T f_1$$
,  $f_1 = z_1 - \hat{V}_D V^T b$  (4.6)

Putting

$$\widetilde{\mathbf{U}}^{\mathbf{T}} \mathbf{f}_{1} = \mathbf{g} \equiv \begin{bmatrix} \mathbf{g}_{1} \\ \mathbf{g}_{2} \end{bmatrix}, \quad \widetilde{\mathbf{U}}^{\mathbf{T}} \mathbf{z}_{1} = \mathbf{w} \equiv \begin{bmatrix} \mathbf{w}_{1} \\ \mathbf{w}_{2} \end{bmatrix}, \quad \mathbf{v}^{\mathbf{T}} \mathbf{b} = \mathbf{c} \equiv \begin{bmatrix} \mathbf{c}_{1} \\ \mathbf{c}_{2} \end{bmatrix} (4.7)$$

and

$$D = \begin{bmatrix} S & O \\ O & O \end{bmatrix} , \tag{4.8}$$

where S is non-singular, then (4.6) becomes

min 
$$g^{T}g$$
,  $g = w - \begin{bmatrix} s & o \\ o & o \end{bmatrix}$  c, (4.9)

and this is solved for any c such that

$$Sc_1 = w_1 \tag{4.10}$$

for which

$$\hat{e}^T \hat{e} = z_2^T z_2 + w_2^T w_2.$$
 (4.11)

 $c_2$  is arbitrary and the solution for which  $b^Tb$  is minimized is called the <u>minimal length</u> solution and is a best linear unbiased estimate of  $\beta$ . Since  $b^Tb = c^Tc$ , this solution is given by

$$c_2 = 0$$
 (4.12)

so that

$$b = V \begin{bmatrix} s^{-1}w_1 \\ 0 \end{bmatrix}$$
,  $s^{-1} = diag(1/d_1)$ . (4.13)

Other solutions, such as the reduced parameter solution, can readily be obtained via the SVD and this allows the decision on the rank of X to be made in the most favourable circumstance. (See for example, Hammarling, 1985, and the references given there.)

# 5. THE GENERAL GAUSS-MARKOV LINEAR MODEL

In this section we look at the general model

$$y = X\beta + e$$
,  $e \in N(O, \sigma^2 W)$ . (5.1)

When W is non-singular this is usually associated with the weighted least-squares problem

min 
$$\hat{e}^T w^{-1} \hat{e}$$
,  $\hat{e} = \hat{y} - \hat{x}b$  (5.2)

If we let F be any matrix for which

$$w = FF^{T}$$
 (5.3)

and put

$$r = F^{-1}\hat{e}$$
 so that  $rcN(O, \sigma^2I)$  (5.4)

then (5.2) becomes

min 
$$r^{T}r$$
,  $r = F^{-1}\hat{y} - F^{-1}\hat{x}b$  (5.5)

which is in the form of the standard problem (2.2), and so we can solve (5.5) as before using the QR factorization and the SVD. But this approach is numerically unstable if W is ill-conditioned and (5.2) and (5.5) are not even defined if W is singular. Adding in artificial noise is a completely unsatisfactory numerical approach for circumventing this.

In place of (5.4) we can let r be any vector such that

$$Fr = \hat{e} \tag{5.6}$$

and rearrange (5.5) to give

min 
$$r^{T}r$$
, subject to:  $\hat{y} = \hat{x}b + Fr$ . (5.7)

While being superficially a trivial rearrangement this has the vital difference of not now requiring non-singularity of F and hence of W. Notice that if

$$r \in N(0,\sigma^2 I)$$
 we still have  $\hat{e} \in N(0,\sigma^2 W)$ 

(5.7) is called the generalized linear least-squares problem. (Paige, 1978.) Tools for the reliable solution of (5.7) are

the QR factorization, the SVD and the generalized singular value decomposition (GSVD). In the next section we indicate how the problem may be solved with the QR factorization and the SVD and in the following section we define the GSVD and give references to its computation and its use in solving (5.7).

# 6. SOLVING THE GENERALIZED LINEAR LEAST-SQUARES PROBLEM

Here we consider the solution of the problem

min 
$$r^{T}r$$
, subject to:  $\hat{y} = \hat{x}b + Fr$  (6.1)

using the QR factorization of (3.1). Denote the QR factorization of  $\hat{X}$  by

$$\hat{X} = Q_{X} \begin{bmatrix} R_{X} \\ Q \end{bmatrix}$$
 (6.2)

and put

$$Q_{\mathbf{x}}^{\mathbf{T}} \hat{\mathbf{y}} = \mathbf{z} = \begin{bmatrix} \mathbf{z}_{1} \\ \mathbf{z}_{2} \end{bmatrix} , Q_{\mathbf{x}} = (Q_{1} Q_{2})$$
 (6.3)

so that (6.1) becomes

min 
$$\mathbf{r}^{\mathrm{T}}\mathbf{r}$$
, subject to:  $\mathbf{z} = \begin{bmatrix} \mathbf{R}_{\mathbf{x}} \\ \mathbf{0} \end{bmatrix} \quad \mathbf{b} + \begin{bmatrix} \mathbf{Q}_{\mathbf{1}}^{\mathrm{T}} \mathbf{F} \\ \mathbf{Q}_{\mathbf{1}}^{\mathrm{T}} \mathbf{F} \end{bmatrix}$  (6.4)

If  $\hat{X}$  does not have full rank we can proceed to compute the SVD of  $R_{\hat{X}}$ , otherwise for any r we can determine b as the solution of the upper triangular equations

$$R_{x}^{b} = z_{1} - (Q_{1}^{T}F)r$$
 (6.5)

so that (6.4) becomes

min 
$$r^T r$$
, subject to:  $z_2 = (Q_2^T F) r$  (6.6)

If we now denote the QR factorization of  $\mathbf{F}^{\mathbf{T}}\mathbf{Q}_2$  as

$$\mathbf{F}^{\mathbf{T}} \mathbf{Q}_{2} = \mathbf{Q}_{\mathbf{F}} \quad \begin{bmatrix} \mathbf{R}_{\mathbf{F}} \\ \mathbf{0} \end{bmatrix}$$
 (6.7)

and put

$$Q_{\mathbf{F}}^{\mathbf{T}} \mathbf{r} = \mathbf{p} \equiv \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \end{bmatrix}$$
 (6.8)

then (6.6) becomes

min 
$$p^{T}p$$
, subject to:  $z_{2} = R_{p}^{T}p_{1}$ . (6.9)

If  $R_F$  does not have full rank we can proceed to compute its SVD, otherwise we can solve the lower triangular system  $R_F^T p_1 = z_2$  for  $p_1$  and hence p is given by

$$R_{F}^{T}p_{1} = z_{2}, p_{2} = 0$$
 (6.10)

so that

$$\mathbf{r}^{\mathrm{T}}\mathbf{r} = \mathbf{p}_{1}^{\mathrm{T}}\mathbf{p}_{1}, \mathbf{r} = \mathbf{Q}_{\mathrm{F}} \begin{bmatrix} \mathbf{p}_{1} \\ \mathbf{0} \end{bmatrix}$$

and b is given from (6.5). Details on this type of approach to the solution of (6.1) are given in Paige (1978, 1979a), error and perturbation analysis in Paige (1979b) and some statistical analysis in Kourouklis and Paige (1981). Further details on the SVD approach are given in Hammarling, Long and Martin (1983).

#### 7. THE GENERALIZED SINGULAR VALUE DECOMPOSITION

To give a gentle introduction to the GSVD we suggest a generalization of the QR factorization of the single matrix to the matrix pair  $(\hat{X},F)$ . We define the generalized QR factorization as

$$\hat{\mathbf{x}} = \mathbf{Q}_{\mathbf{x}} \begin{bmatrix} \mathbf{R}_{\mathbf{x}} \\ \mathbf{O} \end{bmatrix}, \quad \mathbf{Q}_{\mathbf{x}}^{\mathbf{T}} = \mathbf{R}_{\mathbf{F}} \mathbf{Q}_{\mathbf{F}}^{\mathbf{T}},$$
 (7.1)

where Q  $_{\rm X}$  and Q  $_{\rm F}$  are orthogonal and R  $_{\rm X}$  and R  $_{\rm F}$  are upper triangular. If F is non-singular we find that

$$F^{-1}\hat{X} = Q_F \begin{bmatrix} R_F^{-1} R_X \\ Q \end{bmatrix}$$
 (7.2)

which is the QR factorization of  $F^{-1}\hat{x}$ , the data matrix in (5.5). (7.1) gives all the information in (7.2) without relying on invertibility of F and without requiring the numerically damaging step of computing  $F^{-1}\hat{x}$ . Applying this to (6.1) and putting

$$Q_{\mathbf{x}}^{\mathbf{T}}\hat{\mathbf{y}} = \mathbf{z} = \begin{bmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \end{bmatrix}, \quad Q_{\mathbf{F}}^{\mathbf{T}}\mathbf{r} = \mathbf{p} = \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \end{bmatrix}, \quad R_{\mathbf{F}} = \begin{bmatrix} R_{11} & R_{12} \\ \mathbf{p}_2 \end{bmatrix}$$
(7.3)

we get

min 
$$p^{T}p$$
, subject to:  $z = \begin{bmatrix} R_{x} \\ 0 \end{bmatrix}$   $b + R_{F}p$  (7.4)

and if  $R_{x}$  and  $R_{22}$  are of full rank we solve (7.4) as

$$R_{22}p_2 = z_2, p_1 = 0, R_xb = z_1 - R_{12}p_{22}, r^Tr = p_2^Tp_2.$$
 (7.5)

There are variations in the way one can define the GSVD, but the appropriate form for the generalized linear least-squares problem (Paige, 1985) is to define the generalized SVD for the matrix pair  $(\hat{X},F)$  as

$$\hat{\mathbf{X}} = \mathbf{Q} \quad \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix} \quad \begin{bmatrix} \mathbf{I} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{C} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{O} \end{bmatrix} \quad \mathbf{V}^{\mathbf{T}}, \quad \mathbf{F} = \mathbf{Q} \quad \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix} \quad \begin{bmatrix} \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{S} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{I} \end{bmatrix} \quad \mathbf{U}^{\mathbf{T}},$$

$$(7.6)$$

where Q, U and V are orthogonal, R is a non-singular upper triangular matrix and C and S are diagonal with

$$c^2 + s^2 = I$$
,  $c_i > 0$ ,  $s_i > 0$ .

We can choose the diagonal elements of C, the  $c_i$ , to be in descending order, in which case the diagonal elements of S are of course in ascending order. The pairs  $(c_i, s_i)$  are called the generalized singular values of  $(\hat{X}, F)$ .

If F is non-singular then

$$\mathbf{F}^{-1}\hat{\mathbf{x}} = \mathbf{U} \begin{bmatrix} \mathbf{S}^{-1}\mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \quad \mathbf{v}^{\mathrm{T}}, \tag{7.7}$$

which is the SVD of  $F^{-1}\hat{x}$ , and

$$\hat{\mathbf{x}}\hat{\mathbf{x}}^{\mathrm{T}} = (QR) \quad \begin{bmatrix} \mathbf{c}^2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \quad (QR)^{\mathrm{T}}, \quad \mathrm{FF}^{\mathrm{T}} = (QR) \quad \begin{bmatrix} \mathbf{s}^2 & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \quad (QR)^{\mathrm{T}}, \quad (7.8)$$

so that (QR) is the congruence matrix that simultaneously diagonalizes  $\hat{X}\hat{X}^T$  and  ${\rm FF}^T$ . The values  $(c_i^2/s_i^2)$  are the non-zero eigenvalues of the generalized symmetric eigenvalue problem

$$\hat{\mathbf{X}}\hat{\mathbf{X}}^{\mathrm{T}}\mathbf{Z} = \lambda \mathbf{F}\mathbf{F}^{\mathrm{T}}\mathbf{Z}$$
.

For background on the GSVD the reader is strongly recommended to consult Van Loan (1976) and Paige and Saunders (1981).

THE GSVD can readily be applied to (6.1) to yield the solution of the generalized linear least-squares problem and just as the SVD is a valuable tool for the solution and analysis of the standard linear least-squares problem, so the GSVD plays the same role for the generalized problem as is deomstrated in Paige (1985). Stable numerical methods are emerging for computing the GSVD, (Stewart, 1983; Van Loan, 1984; Paige, 1984), the last of these, being based on implicit Kogbetliantz approach, has potential for systolic implementation (Brent, Luk, and Van Loan, 1983.)

## CONCLUSION

We have discussed some of the numerical tools that are necessary for the reliable solution of the general Gauss-Markov linear model and have given references to the details necessary to implement this method. The crux of such methods is the use of orthogonal transformations, which are numerically stable (for example, Wilkinson, 1965), and the avoidance of the numerically damaging steps of forming normal matrices of the form  $\hat{X}^T\hat{X}$  and of matrix inversion.

The Kalman filter can be viewed as a generalized least-squares problem and the ideas here form the basis of reliable and efficient methods for the numerical solution of the Kalman filter problem. (Hammarling, 1985.)

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