МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ
И ВЫЧИСЛИТЕЛЬНЫЕ МЕТОДЫ

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Best Least Square Solution of Boundary Value Problems Associated with a System of First Order Matrix Differential Equation

The best least square solution of the boundary value problem is constructed via modified *QR* algorithm and also *RQ* algorithm. As a result of this work one has a choice of effective methods for finding solutions to two point boundary value problems in the non invertible case. Further these results are exemplified with suitable examples to highlight the modified *QR* and *RQ* algorithms.

Получено решение краевой задачи методом наименьших квадратов с помощью модифицированных *QR* и *RQ* алгоритмов. Предложен способ выбора эффективных методов решения двухточечных краевых задач в случае необратимости. Приведены примеры применения модифицированных *QR* и *RQ* алгоритмов.

K e y w o r d s: boundary value problems, least square solution, QR and RQ algorithms, overdetermined systems, underdetermined systems.

Introduction. In this paper we shall be concerned with the boundary value problem (BVP) associated with first order matrix differential equation of the form

$$y' = A(t)\, y + f\,(t), \quad a \le t \le b, \quad My\,(a) + Ny\,(b) = g, \tag{1}$$

where A is an $(n \times n)$ matrix whose components are continuous functions on $a \le t \le b$, f is an $(n \times 1)$ vector and is continuous. M and N are constant matrixes of order $(m \times n)$ $(m > n)$. Usually one assumes that general differential equations can be written as a first order system $y' = f\,(t, y)$, $a \le t \le b$, where f is continuous on $[a, b] \times R$ and y is a column matrix with components $(y_1, y_2, ..., y_n)^T$. The interval ends a and b are finite or infinite constants. For linear problems, the ordinary differential equation takes the form

$$y' = A(t)\, y + f(t). \tag{2}$$

The linear homogeneous system associated with (2) is

$$y' = A(t)\, y. \tag{3}$$

If Y is a fundamental matrix of the homogeneous system (3), then any solution of (3) is of the form $y(t) = Y(t)\,C$ where C is a constant $(n \times 1)$ vector. If y is any solution of (2) and $\bar{y}$ is a particular solution of (2), then $(y - y^{-})$ is a solution (3). Thus [1] $y - \bar{y} = Y(t)\,C$ or $y(t) = \bar{y}(t) + Y(t)\,C$. A particular solution $\bar{y}(t)$ of (2) is given by

$$\bar{y}(t) = Y(t) \int_a^t Y^{-1}(s)\, f(s)\, ds.$$

Thus

$$Y(t) = Y(t)\, C + Y(t) \int_a^t Y^{-1}(s)\, f(s)\, ds. \tag{4}$$

Substituting the general form of $y(t)$ in the boundary condition matrix in (1), we get

$$[MY(a) + NY(b)]C + NY(b) \int_a^b Y^{-1}(s)\, f(s)\, ds = g.$$

If we denote the characteristic matrix D by $D = MY(a) + NY(b)$, then

$$DC = -NY(b) \int_a^b Y^{-1}(s)\, f(s)\, ds + g.$$

If D is non-singular, then C can be determined uniquely, and in this case

$$C = -D^{-1} NY(b) \int_a^b Y^{-1}(s)\, f(s)\, ds + D^{-1} g.$$

Substituting the general form of C in (4), we get

$$y(t) = -Y(t)\, D^{-1} NY(b) \int_a^b Y^{-1}(s)\, f(s)\, ds + Y(t) \int_a^t Y^{-1}(s)\, f(s)\, ds + D^{-1} g =$$

$$= \int_a^b G(t,s)\, f(s)\, ds + D^{-1} g,$$

where G is the Green's function for the homogeneous BVP and is given by

$$G(t,s) = \left\{ \begin{array}{l} Y(t)\, D^{-1} MY(a)\, Y^{-1}(s), \; a \le t \le s \le b \\ -Y(t)\, D^{-1} MY(a)\, Y^{-1}(s), \; a \le s \le t \le b \end{array} \right\}.$$

If D is an $(m\times n)$ matrix and rank $(D) = r < m$, then the system

$$DC = b, \tag{5}$$

where

$$b = -NY(b)\int_a^b Y^{-1}(s)\, f(s)\, ds + g(t)$$

possesses a solution only in the least square sense.

Least Square Solution of Over Determine Systems. If D is an $(m\times n)$ matrix with rank $(D) = r < m$, then the system of equations (5) is called an overdetermined system. We now attempt to solve the system by the method of least squares i.e., determine C to minimize $\|DC - b\|_z$. If rank of D is n (i.e., columns of D are L I.), then $D^T DC = D^T b$. Note that $D^T D$ is positive definite matrix and $C = (D^T D)^{-1} D^T b$.

However, the algorithm resulting from forming and solving (5) is not as numerically stable as the alternating way of using QU decomposition [2, 3]. If $r < n$, then $D^T D$ is singular and (5) cannot be solved directly. In this case, the solution is not unique. A solution of (5) in this case is given by $C = D^+ b$, where D^+ is the psuedo inverse of D. The unique distinction of the above equation is that C is the unique solution of (5) in the least square sense.

Example 1. Consider the linear system of equations:

$$x_1 - x_2 + x_3 = 1.0,$$
$$x_1 - 0.5x_2 + 0.25x_3 = 0.5,$$
$$x_1 - 0.0x_2 + 0.0x_3 = 0.0,$$
$$x_1 + 0.5x_2 + 0.25x_3 = 0.5,$$
$$x_1 + x_2 + x_3 = 2.0.$$

The above system of equations can be put in the form

$$\begin{bmatrix} 1 & -1.0 & 1.0 \\ 1 & -0.5 & 0.25 \\ 1 & 0.0 & 0.0 \\ 1 & 0.5 & 0.25 \\ 1 & 1.0 & 1.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.0 \\ 0.5 \\ 0.0 \\ 0.5 \\ 2.0 \end{bmatrix},$$

$$DC = b, \tag{6}$$

Since D is 5×3 matrix of rank 3 .We multiply the equation (6) by D^T and get $D^T DC = D^T b$ and hence $C = (D^T D)^{-1} D^T b$, and C is unique. In general, if the matrix D is rectangular (or singular), then the equation (6) can have either an infinite number of solutions or no solution. If D is singular and $R(D)$ and $N(D)$ represent the range and null space of D, respectively, then (6) will have solutions if $b \in R(D)$. In this case, if C is any n vector in $N(D)$ and $\overline{C}_0$ is any solution of (6), then the vector $C + \overline{C}_0$ will also be a solution. If $b \notin R(D)$, then the system (6) will not have a solution.

Further, if D is an $(m \times n)$ matrix, then for a given $D \in C^{m \times n}$ and b € C^m, the linear system (6) is consistent if and only if $b \in R(D)$. Otherwise the residual vector

$$r = b - DC \tag{7}$$

is non-zero for all $C \in C^n$, and it may be desired to find an appropriate solution of (6), by which we mean a vector C, making the residual vector in (7) very close to zero in some sense. The following theorem shows that $\|DC - b\|$ is minimized by choosing $C = D^+ b$, where D^+ is such that

$$D^+ DD^+ = D^+, \tag{8}$$

$$DD^+ D = D, \tag{9}$$

$$(DD^+)^* = DD^+, \tag{10}$$

$$(D^+ D)^* = D^+ D \tag{11}$$

such a D^+ is unique. If D^+ satisfies conditions (9) and (10), then D^+ need not be unique.

Theorem 1. Let $D \in C^{m \times n}$ and $b \in C^m$. Then $\|DC - b\|$ is the smallest when $C = D^+ b$ where D^+ satisfies (9) and (10). Conversely, if D^+ has property that for all b, $\|DC - b\|$ is the smallest when $C = D^+ b$, then D^+ satisfies (9) and (10).

P r o o f. If $P_{R(D)}$ is the projection matrix on $R(D)$, then write $DC - b = (DC - P_{R(D)} b) + (P_{R(D)} b - b)$. Then

$$\|DC - b\|^2 = \|DC - P_{R(D)} b\|^2 + \|P_{R(D)} b - b\|^2 . \tag{12}$$

Since $(DC - P_{R(D)} b) \in R(D)$ and $-(I - P_{R(D)})\, b \in R(D)$, it follows that (12) assumes minimum value if, and only if

$$DC = P_{R(D)} b, \tag{13}$$

which certainly holds, if $C = D^T b$ for any D^+ satisfying (9) and (10). Hence $DD^+ = P_{R(D)}$. Conversely, if D^+ is such that for all b, $\|DC - b\|$ is the smallest when $C = D^+ b$, then by (13), we have $DD^+ b = P_{R(D)} b \vee b$, and hence $DD^+ = P_{R(D)}$. Thus, D^+ satisfies (9) and (10). Suppose D^+ satisfies (8) and (11), then we have the following theorem.

Theorem 2. Let $D \in C^{m\times n}$ and $b \in C^m$. If $DC = b$ has a solution for C, the unique solution for which $\|C\|$ is the smallest is given by $C = D^+ b$, where D^+ satisfies conditions (8) and (11). Conversely, if $D^+ \in C^{n\times m}$, $C^{n\times m}$ is such that, whenever $DC = b$ has solution $C = D^+ b$ is the solution of minimum norm, then D^+ satisfies (8) and (11).

P r o o f. The proof is similar to the proof of the Theorem 1.

Theorem 3. Let $D \in C^{m\times n}$ and $b \in C^m$. If $DC = b$ has a solution for C, then the unique solution of $DC = b$ is $C = D^+ b$, where D^+ satisfies (8)-(11).

Lemma. Let $D \in C^{m\times n}$. Then D is one–one mapping of $R(D^*)$ onto $R(D)$.

Corollary. Let $D \in C^{m\times n}$, $b \in R(D)$. Then there is a unique minimum norm solution of

$$DC = b, \tag{14}$$

which lies in $R(D^*)$.

P r o o f. By lemma, the equation (14) has a unique solution C_o in $R(D^*)$. Now the general solution is given by $C = C_0 + C_1$ for some $C_1 \in N(D)$. Clearly, $\|C_0\|^2 = \|C_0\|^2 + \|y\|$, proving that $\|C\|^2 \geq \|C_0\|^2$ and equality holds, only if $C = C_0$.

Non-invertible BVP occur in a natural way in the study of bifurcation, in singular perturbation theory, and in nonlinear eigenvalue problems. A similar situation arises in some identification problems, which often leads to undetermined two-point BVP. In such situations one normally seeks solutions which satisfy the boundary conditions exactly and solve the differential equation in some least square sense.

Definition 1. For a given $f \in C^n[a,b]$, the set of all least square solutions of (1) is defined as

$$S_f = \left\{ x \in D(L) \mid \|Lx - f\| = \underset{y \in D(L)}{Inf} \|Ly - f\| \right\},$$

where $D(L)$ is the domain of the operator L and is given by $D(L) = BC'^n[a,b]$, $BC'^n[a,b]$ is the subspace of $C'^n[a,b]$ satisfies the boundary conditions in (1).

Definition 2. The best least square solution (1) is denoted by y^+ and is defined to be an element of S_f of minimum norm (if such exists) i.e., $\|y^+\| = \min\limits_{x \in S_f} \|x\|$.

We now present an algorithm for computing the minimal norm least square solution of the general system of equations $Ax = b$, where A is an $(m\times n)$ matrix and x is column matrix with components $(x_1, x_2, ..., x_n)^T$ and $b = (b_1, b_2, ..., b_n)^T$.

Q-R Decomposition. In this section we first present QR algorithm and then present our main result on modified QR algorithm, when the matrix A is of rank

$p = \min(m, n)$. The algorithm presented here depends upon the rank factorization of the form $AP = \mathrm{QR}$, where P is an $(n \times m)$ permutation matrix such that the first p columns of AP are linearly independent. Q is an $(m\times n)$ matrix with orthonormal columns ($Q^T Q = I$) and R is an upper trapezoidal matrix of rank p. We shall denote $lm\,(A) = \{Ax \in R^m | \, x \in R^n\}$ the column space of A and $Ker\,(A) = = \{x \in R^n \,|\, Ax = 0\}$. We first present QR-algorithm.

Theorem 4. Let A be an $(m\times n)$ matrix with rank n $(m \geq n)$ then there exists a unique $(m\times n)$ orthogonal matrix Q $(Q^T Q = In)$ and a unique $(n \times n)$ upper triangular matrix R with positive diagonal elements ($r_{ii} > 0$) such that $A = QR$.

P r o o f. It may be noted that the theorem is a restatement of the Gram-Schmidt orthogonalization process. If we apply Gram-Schmidt to the columns of $A = [a_1, a_2, ..., a_n]$ from left to right, we get a sequence of orthonormal vectors q_1 through q_n spanning the same space and these orthogonal vectors are the columns of Q. Further, Gram-Schmidt also computes coefficient $r_{ii} = q_j^T a_i$ expressing each column a_i as a linear combination of q_1 through q_i: $ai = \sum_{j=1}^{n} r_{ji} q_j$. These r_{ji} are the just entries of R.

We shall now present the classical Gram-Schmidt and modified Gram-Schmidt algorithms for factoring of $A = QR$:

For i =1 to n /* compute the ith column of Q and R*/

$q_i = a_i$

for j = 1 to i – 1 /*subtract component in q_j direction from a_i*/

$r_{ji} = q_j^T a_i CGS$

$r_{ji} = q_j^T q_i \, MGS$

$q_i = q_i - r_{ji} q_j$

end for

$r_{ii} = \|q_i\|_2$.

If $r_{ii} = 0$ /* a_i is linearly independent of $a_1, a_2, ..., a_{i-1}$,*/

quit

end if

$q_i = \dfrac{q_i}{r_{ii}}$

end for.

We further need the following results for construction of the least square algorithm and the best least square algorithm.

Result 1. Let A be given $(m\times n)$ matrix of rank p. Then there exists a factorization $AP = QR$ with the following properties:

(i) p is an $(n\times n)$ permutation matrix with first p columns of AP form a basis for Im (A) and

(ii) Q is an $(m\times p)$ matrix with orthogonal columns and R is a $(p\times n)$ upper-trapezoidal matrix of the form $R = [R_1, R_2]$,where R_1 is non-singular $(p\times p)$ upper triangular matrix and R_2 is a $(p\times n-p)$ matrix [4].

Result 2. Let A be an $(m\times n)$ matrix with rank p = $\min\{m, n\}$.Write $A=[a_1, a_2, ..., a_n]$, where $a_j \in R^m$ and p be an $(n\times n)$ permutation matrix such that $AP = QR$, where Q is an $(m\times p)$ matrix with orthonormal columns and R is an $(p\times n)$ upper trapezoidal of rank p. Then the first p columns of AP are linearly independent and all the least square solutions of the system $Ax = b$ can be obtained by solving the consistent system: $RP^T x=Q^* b$. If we write $R = [R_1, R_2]$, R_1 is $(p\times p)$ upper triangular, then $\bar{x}=P\begin{bmatrix} u \\ v \end{bmatrix}\begin{matrix} p\} \\ n-p\} \end{matrix}$, where $V\in R^{n-p}$ is arbitrary and $u=R_1^{-1}(a^* b-R_2 v)$ are the least square solutions of $Ax = b$. A basic least square solution is obtained by taking $v = 0$.

Let A be an $(m\times n)$ matrix and $b\in R^m$ be given. Let rank of A be $p\le \min\{m, n\}$.The following is the algorithm to compute the least square solution. We use the following notation

$a_{ij} : = b_{ij}$ means a_{ij} becomes b_{ij} for all i = 1 to m and j = 1 to n.

A l g o r i t h m:

$q_{ij} := a_{ij}$, $i=1$ to m; $j=1$ to n;

$r_{ij} := 0$, $i=1$ to m; $j=1$ to $n+1$;

$s_j := j$, $j=1$ to n;

$p := n$;

for $k=1$ to n;

$\delta_j = |q_{ij}|^2, \sum_{i=1}^{m} |q_{ij}|^2, \quad i=k,...,n,$

compute index c, $k\le c\le n$ such that $\delta c=\max\limits_{1\le j\le n}\delta_j$,

if $\delta c=0$ go to 20,

$20 : p : k-1$ go to 30,

interchange column K of Q with column C of Q,

interchange column K of R with column C of R

interchange number δk with number δc,

interchange index s_k with index C

$r_{kk} := \sqrt{\delta k}$

$q_k := q_k / r_{kk}$

$r_{kj} = q_k^* q_j$, $j=k+1,...,n$

$q_j = q_j - r_{kj} q_k$, $j=k+1,...,n$

$r_{k,n+i} = q_k^* b$

30 : for $j = p + 1$ to n

$x_j = 0;$

Back solve the system of equations

$r_{11}x_1 + ... + r_{1p}x_p = r_{1,n+1}$

$r_{22}x_{12} + ... + r_{2p}x_p = r_{2,n+1}$

....

$r_{pp}x_p = r_{p,n+1}$

to determine $x_1, x_2, ..., x_p$

for $j = n, n-1, \dots, 1$

$k = s_j$.

If $k \neq j$ $x_k \leftrightarrow x_j$, $x = [x_1, x_2, ..., x_n]$ is the least square solution of $Ax = b$.

Algorithm for MINLS. If $p = n$ STOP, the least square solution already found is the minimal norm least square solution of $Ax = b$:

else $v := n - p$

$b_j := x_j, j = 1$ to n

$x_j := 0, j = p + 1$ to n

for $k = p + 1$ to n

$x_k := 1$

Back solve the equation systems $Rx = 0$ to determine $x_1, x_2, ..., x_p$

$J := k - p$

$a_{ij} := x_i$ for $i = 1$ to n

$x_k := 0$

for $i = n$ to 1

$k := s_i$,

if $k \neq i$ interchange a_{kj} and a_{ij} for $j = 1$ to v.

Computation of Pseudoinverse. Algorithm min Ls can be used to find pseudoinverse of an $(m \times n)$ matrix A. Using min Ls algorithm m times, solve for a_i^+ of the problem $Ax = e_i$, where e_i $(1 \leq i \leq m)$ are the standard Eucledian basis for R^m. Then the Pseudoinverse of the matrix A denoted by A^+ is given by $A^+ = \{a_1^*, a_2^*, ..., a_n^*\}$. To illustrate the results mentioned above, we consider the system of equations of the form $y' = A(t)\, y + f$, satisfying

$$My(0) + Ny(1) = b, \tag{15}$$

where

$$A = \begin{bmatrix} 0 & 1 & t \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad f(t) = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix},$$

$$M=\begin{bmatrix}1 & 2 & 3\\ 1 & 5 & 6\\ 1 & 8 & 9\\ 1 & 11 & 12\end{bmatrix},\quad N=\begin{bmatrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 1 & 1\end{bmatrix},\quad b(t)=\begin{bmatrix}7\\ 13.5\\ 19.5\\ 20.5\end{bmatrix}.$$

A fundamental matrix of the homogeneous system $y'=Ay$ is given by

$$Y(t)=\begin{bmatrix}1 & t & t^2\\ 0 & 1 & t\\ 0 & 0 & 1\end{bmatrix}.$$

Substituting the general form of the solution $y(t) = Y(t)C$ in the boundary condition matrix $My(0) + Ny(1) = g$, we get

$$DC=-NY(1)\int_0^1 Y^{-1}(s)\,f(s)\,ds+g,$$

where

$$D=\begin{bmatrix}1 & 2 & 3\\ 1 & 5 & 6\\ 1 & 8 & 9\\ 1 & 11 & 12\end{bmatrix}$$

and the right hand side is given by $[6, 13, 19, 24]^T = b$ or $DC = b$. Here D is a (4×3) matrix of rank 2. The minimal norm least squares solution of this system as determined by the algorithm MINLS is given by $C=[1\quad 0.5\quad 1.5]^T$ with the least square residual equal to 1.

The best least square solution $y^{+}(t)$ of BVP (15) is as follows

$$y^{+}(t)=y(t)C+y(t)\int_a^t y^{-1}(s)\,f(s)\,ds=\begin{bmatrix}1+\frac{1}{2}+t^2+t^2\\ \frac{1}{2}+t+t^2\\ \frac{3}{2}+t\end{bmatrix}.$$

Example 2. Consider BVP $y'=Ay+f$. $My(0) + Ny(1) = g$, where

$$A=\begin{bmatrix}0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{bmatrix},\quad f=\begin{pmatrix}0\\ 0\\ 0\\ 1\end{pmatrix},\quad g=\begin{bmatrix}\frac{4}{3} & -\frac{75}{24} & \frac{125}{24}\end{bmatrix}^T,$$

$$M=\begin{bmatrix} -1 & 1 & 0 & \frac{1}{2} \\ 1 & 1 & 1 & -1 \\ 0 & 2 & -2 & \frac{2}{3} \end{bmatrix}, \quad N=\begin{bmatrix} 2 & 0 & \frac{1}{2} & -1 \\ 1 & 4 & 0 & \frac{7}{6} \\ 1 & 0 & \frac{1}{2} & 0 \end{bmatrix}.$$

A fundamental matrix Y of $y'=Ay$ is given by

$$Y(t)=\begin{bmatrix} 1 & t & t^2 & t^2 \\ 0 & 0 & 2t & 3t^2 \\ 0 & 0 & 2 & 6t \\ 0 & 0 & 0 & 6 \end{bmatrix}, \quad Y^{-1}(t)=\begin{bmatrix} 1 & -t & \frac{1}{2}t^2 & -\frac{1}{6}t^2 \\ 0 & 1 & -t & \frac{1}{2}t^2 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2}t \\ 0 & 0 & 0 & \frac{1}{6} \end{bmatrix}.$$

Substituting the general form solution $Y(t)\,C$ in the boundary condition matrix, we get

$$\begin{bmatrix} 1 & 3 & 3 & 2 \\ 2 & 6 & g & 5 \\ 1 & 3 & -3 & 0 \end{bmatrix} C = -\begin{bmatrix} 2 & 0 & \frac{1}{2} & -1 \\ 1 & 4 & 0 & \frac{7}{6} \\ 1 & 0 & \frac{1}{2} & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 2 & 6 \\ 0 & 0 & 0 & 6 \end{bmatrix} =$$

$$=\int_0^1 \begin{bmatrix} 1 & -s & \frac{1}{2}s^2 & -\frac{1}{6}s^2 \\ 0 & 1 & -s & \frac{1}{2}s^2 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2}s \\ 0 & 0 & 0 & \frac{1}{6} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} ds + g = \begin{bmatrix} \frac{1}{3} \\ \frac{45}{24} \\ \frac{7}{24} \end{bmatrix} + \begin{bmatrix} \frac{4}{3} \\ -\frac{75}{24} \\ \frac{127}{24} \end{bmatrix} = -\begin{bmatrix} 1 \\ 5 \\ -5 \end{bmatrix}.$$

This is an underdetermined system and hence algorithm MINLS chooses the minimal norm solution amongst all the solutions of the problem. The minimal norm least square solution determined by the MINLS algorithm is $C=[-0.211009174 \quad -0.633027523 \quad 0.963302752 \quad 0.110091743]^T$. Slight alterations of this program will handle the complex case, as the algorithm we presented is for the real data. Note that we compiled the MINLS incorporating Algorithm of least squares in IBMAT.

***QR* Factorization via Gram-Schmidt.** $Ax = b$, write $A = QR$, where Q is unitary and R is upper triangular, Q is $m\times m$ and R is $m\times n$ $(m\geq n)$. Since $m\geq n$ the last m-n rows of R will be zero. We first start with a_1. Write

$$a_1 = q_1 r_{11} \Rightarrow q_1 = a_1 / r_{11}, \tag{16}$$

$$a_2 = q_1 r_{12} + q_2 r_{22} \Rightarrow q_2 = \frac{a_2 - r_{12} q_1}{r_{22}}, \tag{17}$$

. . . .

$$a_2 = q_1 r_{1n} + q_2 r_{2n} + \ldots + q_n r_{nn} \Rightarrow q_n = \frac{a_n \sum_{i=1}^{n} r_{in} q_0}{r_{nn}}, \tag{18}$$

since the columns of a_j of A are given, we need to determine the columns q_j of Q and entries r_{ij} of R such that Q is orthonormal, i.e.,

$$q_i^* q_j = \delta_{ij}, \tag{19}$$

and R is upper triangular and $A = QR$. The latter two conditions are already reflected in the above formulae using (16) in (19) , we get $q_1^* q_1 = \frac{a_1^* a_1}{r_{11}^2} = 1$ so that $r_{11} = \sqrt{a_1^* a_1} = \|a_1\|_2$. Note that, we choose arbitrarily the positive square root so that the factorization becomes unique.

From (18) we have $q_1^* q_2 = 0$, $q_2^* q_2 = 1$. Applying (17) we get

$$q_1^* q_2 = \frac{q_1^* a_2 - r_{12} q_1^* q_1}{r_{22}} = 0 .$$

Thus

$$q_2 = \frac{a_2 - ([q]_1^* a_2)\, q_1}{r_{22}}$$

(since $q_1^* q_1 = 1,\ r_{12} = q_1^* a_2$). Now to find r_{22} we normalize $\|q_2\|_2 = 1$. Thus $r_{22} = \| a_2 - (q_1^* a_2)\, q_1\|_2$. For $n = 3$ we have $q_1^* q_3 = 0, q_2^* q_3 = 0, q_3^* q_3 = 1$. The first two of the above conditions together with (18) for $n = 3$ yield

$$q_1^* q_3 = \frac{q_1^* a_3 - r_{13} q_1^* q_1 - r_{23} q_1^* q_2}{r_{33}} = 0 .$$

Since $q_1^* q_2 = 0$ and $q_1^* q_1 = 1$, we have $r_{13} = q_1^* a_3$. Similarly $q_2^* q_3 = 0$ and (18) for $n = 3$ again yields

$$q_2^* q_3 = \frac{q_2^* a_3 - r_{13} q_2^* q_1 - r_{23} q_2^* q_2}{r_{33}} = 0$$

so that $r_\downarrow 23 = q_\downarrow 2^\uparrow * a_\downarrow (3) (\therefore q_\downarrow 2^\uparrow * q_\downarrow 1 = 0$ and $q_\downarrow 2^\uparrow * \; q_\downarrow 2 = 1)$. Further $q_3^* q_3 = \|q_3\|_2 = 1$, we get

$$q_3 = \frac{a_3 - (q_1^* a_3)\, q_1 - (q_2^* a_3)\, q_2}{r_{33}}, \quad r_{33} = \| a_3 - (q_1^* a_3)\, q_1 - (q_2^* a_3)\, q_2 \|_2 .$$

In general we have the following algorithm $r_{ij} = q_1^* a_j \; (i \neq j)$:

$$v_j = a_j - \sum_{i=1}^{j-1} r_{ij} q_i, \quad r_{jj} = \| v_j \|_2, \quad q_j = \frac{v_j}{r_{jj}} .$$

The following is the classical Gram-Schmidt algorithm:

for $j = 1$ to n
$v_j = a_j$;
for $i = 1 : j - 1$
$r_{ij} = q_1^* a_j, \; v_j = v_j - r_{ij} q_i$
end
$r_{jj} = \| v_j \|_2, \; q_j = \dfrac{v_j}{r_{jj}}$
end.

Example 3. Consider $\begin{bmatrix} 1 & 2 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} x = b$. First $v_1 = a_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$ and $r_{11} = \| v_1 \| = \sqrt{2}$.

This gives $q_1 = \dfrac{v_1}{\| v_1 \|} = \dfrac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$. Next,

$$v_2 = a_2 - (q_1^* a_2)\, q_1 = a_2 - r_{12} = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} - \frac{\sqrt{2}}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} .$$

Thus $r_{12} = 2/\sqrt{2} = \sqrt{2}$. Moreover, $r_{22} = \|v_2\|_2 = \sqrt{3}$ and

$$q_2 = \frac{v_2}{\|v_2\|} = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}.$$

In the last iteration we have $r_2 = a_2 - (q_1^* a_2)\, q_1 - (q_2^* a_2)\, q_2$, where $(q_1^* a_3)\, q_1 = r_{13}$ and $([q]_2^* a_3)\, q_3 = r_{23}$. From this we compute $r_{13} = 1/\sqrt{2}$ and $r_{23} = 0$. This gives

$$v_3 = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} - \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} - 0 = \frac{1}{2} \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}.$$

Finally, $r_{33} = \|v_3\|_2 = \sqrt{6}/2$ and $q_3 = \dfrac{v_3}{\|v_3\|_2} = \dfrac{1}{\sqrt{6}} \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}$. Thus

$$Q = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \end{bmatrix}, \quad R = \begin{bmatrix} \sqrt{2} & \sqrt{2} & \frac{1}{\sqrt{2}} \\ 0 & \sqrt{3} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{2} \end{bmatrix}.$$

Generalized *QR* Factorization. In this section we shall be concerned with the system of equations $Ax = b$, where A is an $(n \times m)$ matrix and x is an $(m \times 1)$ vector we assume that $n \le m$. This is an underdetermined system. The QR-factorization of $(n \times m)$ matrix A can be written as $A = QR$, where Q is an $(n \times n)$ orthonormal matrix and $R = Q^T A$ is zero below the main diagonal and is given by $R = Q^T A = \begin{bmatrix} R_{11} \\ 0 \end{bmatrix}$, where R_{11} is an $(n \times n)$ upper triangular matrix. If $n < m$ then the QR factorization of A assumes $Q^T A = [R_{11} \quad R_{12}]$, where R_{11} is an $(n \times n)$ upper triangular matrix. However in many practical applications it will be more appropriate to write A in the form $A = [0 \quad R_{11}]\, Q$, which is known as RQ factorization. In fact QR and RQ factorization are the QL and LQ factorization and are in fact orthogonal — lower-triangular (QL) and lower triangular — orthogonal factorization (LQ). It is well known in fact that the orthogonal factors of A provide information about its column and row spaces. If rank of A is $k \le \min\{n, m\}$, then there exist orthonormal matrix Q and a permutation matrix P such that

$$Q^T AP = \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix},$$

$$R_{11} \text{ being } k\times k,\ R_{12} \text{ being } (m-k)\times k,$$

$$\mathbf{o} \text{ being } k\times(n-k) \text{ and } \mathbf{o} \text{ being } (m-k)\times(n-k),$$

where R_{11} is a $(k\times k)$ upper triangular matrix and R_{11} is non singular we present generalized RQ factorization for the system of equations $Ax = b$.

Let A be an $(n\times m)$ matrix and assume that $n < m$. Then there exists orthogonal matrix Q $(n\times n)$ and U $(m\times m)$ such that $Q^T AU = R$, where $R = [0 \quad R_{11}]$, $\mathbf{o}$ being $(m-n)\times n$ and R_{11} being $(n\times n)$ matrix, and further R_{11}, being upper triangular, is non-singular. By QR-factorization with column pivoting of A, we have

$$Q^T AP = \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix},$$

$$R_{11} \text{ being } q\times q,\ R_{12} \text{ being } (m-q)\times q,$$

$$\mathbf{o} \text{ being } q\times(n-q) \text{ and } \mathbf{o} \text{ being } (m-q)\times(n-q),$$

where q = rank (A).

Отримано найкращий розв’язок крайової задачі методом найменших квадратів за допомогою модифікованих QR та RQ алгоритмів. Запропоновано спосіб вибору ефективного методу розв’язування двохточкових крайових задач у випадку необоротності матриці. Наведено приклади застосування модифікованих QR та RQ алгоритмів.

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