

(2.12) Example.

Compute  $\text{EGP}(A)$  where:

$$A = \begin{bmatrix} 1, & 1, & 0, & 0; \\ 2, & 2, & 1, & 0; \\ -2, & 0, & 0, & -1; \\ -1, & 1, & 2, & -1 \end{bmatrix}$$

(\*)  $A_1 = A;$

(\*)  $k = 1; A_1(1,1) \neq 0 \Rightarrow P_1 = I; T_1 = P_1 A_1;$

$$H_1 = \begin{bmatrix} 1, & 0, & 0, & 0; \\ \lambda_2, & 1, & 0, & 0; \\ \lambda_3, & 0, & 1, & 0; \\ \lambda_4, & 0, & 0, & 1 \end{bmatrix}$$

The values  $\lambda_2, \lambda_3, \lambda_4$  are determined by requiring that the elements (2,1), (3,1) and (4,1) - that is, the elements of the k-th column below the diagonal - in the matrix  $H_1 T_1$  be equal to zero:

$$\lambda_2 T_1(1,1) + T_1(2,1) = 0 \quad ; \quad \lambda_3 T_1(1,1) + T_1(3,1) = 0 \quad ; \quad \lambda_4 T_1(1,1) + T_1(4,1) = 0$$

Considering that  $T_1(1,1) \neq 0$ , the values  $\lambda_2, \lambda_3, \lambda_4$  are *uniquely determined*:

$$\lambda_2 = - \frac{T_1(2,1)}{T_1(1,1)} = -2 \quad ; \quad \lambda_3 = - \frac{T_1(3,1)}{T_1(1,1)} = 2 \quad ; \quad \lambda_4 = - \frac{T_1(4,1)}{T_1(1,1)} = 1$$

Finally:

$$\begin{bmatrix} 1, & 0, & 0, & 0; \\ -2, & 1, & 0, & 0; \\ 2, & 0, & 1, & 0; \\ 1, & 0, & 0, & 1 \end{bmatrix} \begin{bmatrix} 1, & 1, & 0, & 0; \\ 2, & 2, & 1, & 0; \\ -2, & 0, & 0, & -1; \\ -1, & 1, & 2, & -1 \end{bmatrix} = \begin{bmatrix} 1, & 1, & 0, & 0; \\ 0, & 0, & 1, & 0; \\ 0, & 2, & 0, & -1; \\ 0, & 2, & 2, & -1 \end{bmatrix}$$

$$H_1 \quad T_1 \quad = \quad A_2$$

(\*)  $k = 2; A_2(2,2) = 0 \Rightarrow$  since  $A_2(3,2) \neq 0$ , we swap row two and row three:  $P_2 = P_{2,3};$

$$\begin{bmatrix} 1, & 0, & 0, & 0; \\ 0, & 0, & 1, & 0; \\ 0, & 1, & 0, & 0; \\ 0, & 0, & 0, & 1 \end{bmatrix} \begin{bmatrix} 1, & 1, & 0, & 0; \\ 0, & 0, & 1, & 0; \\ 0, & 2, & 0, & -1; \\ 0, & 2, & 2, & -1 \end{bmatrix} = \begin{bmatrix} 1, & 1, & 0, & 0; \\ 0, & 2, & 0, & -1; \\ 0, & 0, & 1, & 0; \\ 0, & 2, & 2, & -1 \end{bmatrix}$$

$$P_{2,3} \quad A_2 \quad = \quad T_2$$

so that  $T_2(2,2) \neq 0$ .

Then:

$$H_2 = \begin{bmatrix} 1, & 0, & 0, & 0; \\ 0, & 1, & 0, & 0; \\ 0, & \lambda_3, & 1, & 0; \\ 0, & \lambda_4, & 0, & 1 \end{bmatrix}$$

The values  $\lambda_3, \lambda_4$  are determined by requiring that the elements (3,2), and (4,2) - that is, the elements of the k-th column below the diagonal - in the matrix  $H_2 T_2$  be *equal to zero*:

$$\lambda_3 T_2(2,2) + T_2(3,2) = 0 \quad ; \quad \lambda_4 T_2(2,2) + T_2(4,2) = 0$$

Considering that  $T_2(2,2) \neq 0$ , the values  $\lambda_3, \lambda_4$  are *uniquely determined*:

$$\lambda_3 = - \frac{T_2(3,2)}{T_2(2,2)} = 0 \quad ; \quad \lambda_4 = - \frac{T_2(4,2)}{T_2(2,2)} = -1$$

Finally:

$$\begin{bmatrix} 1, & 0, & 0, & 0; \\ 0, & 1, & 0, & 0; \\ 0, & 0, & 1, & 0; \\ 0, & -1, & 0, & 1 \end{bmatrix} \begin{bmatrix} 1, & 1, & 0, & 0; \\ 0, & 2, & 0, & -1; \\ 0, & 0, & 1, & 0; \\ 0, & 2, & 2, & -1 \end{bmatrix} = \begin{bmatrix} 1, & 1, & 0, & 0; \\ 0, & 2, & 0, & -1; \\ 0, & 0, & 1, & 0; \\ 0, & 0, & 2, & 0 \end{bmatrix}$$

$$H_2 \quad T_2 \quad = \quad A_3$$

(\*)  $k = 3$ ;  $A_3(3,3) \neq 0 \Rightarrow P_3 = I$ ;  $T_3 = A_3$ ;

$$H_3 = \begin{bmatrix} 1, & 0, & 0, & 0; \\ 0, & 1, & 0, & 0; \\ 0, & 0, & 1, & 0; \\ 0, & 0, & \lambda_4, & 1 \end{bmatrix}$$

The value  $\lambda_4$  is determined by the requirement that the element (4,3) - that is, the elements of the k-th column below the diagonal - in the matrix  $H_3 T_3$  be *equal to zero*:

$$\lambda_4 T_3(3,3) + T_3(4,3) = 0$$

Considering that  $T_3(3,3) \neq 0$ , the value  $\lambda_4$  is *uniquely determined*:

$$\lambda_4 = - \frac{T_3(4,3)}{T_3(3,3)} = -2$$

Finally:

$$\begin{bmatrix} 1, & 0, & 0, & 0; \\ 0, & 1, & 0, & 0; \\ 0, & 0, & 1, & 0; \\ 0, & 0, & -2, & 1 \end{bmatrix} \begin{bmatrix} 1, & 1, & 0, & 0; \\ 0, & 2, & 0, & -1; \\ 0, & 0, & 1, & 0; \\ 0, & 0, & 2, & 0 \end{bmatrix} = \begin{bmatrix} 1, & 1, & 0, & 0; \\ 0, & 2, & 0, & -1; \\ 0, & 0, & 1, & 0; \\ 0, & 0, & 0, & 0 \end{bmatrix}$$

$$H_3 \quad T_3 \quad = \quad A_4$$

(\*)  $D = A_4$ ;  $P = P_3 P_2 P_1 = P_{2,3}$ ;

Then:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ -2 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 2 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 0 & 1 & 0 \\ -2 & 1 & 0 & 0 \\ -1 & 1 & 2 & 1 \end{bmatrix}$$

 $H_1^{-1}$  $P_{2,3}^t$  $H_2^{-1}$  $H_3^{-1}$  $\Sigma$ 

and then:

$$S = P \Sigma = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 \\ -1 & 1 & 2 & 1 \end{bmatrix}$$

The elements  $T_1(1,1)$ ,  $T_2(2,2)$  and  $T_3(3,3)$  used to derive the elementary Gaussian matrices  $H_1$ ,  $H_2$  and  $H_3$  (in general, the element  $T_k(k,k)$  used to derive the matrix  $H_k$ ) are called *pivots*. The term *pivoting* refers to the exchanges made at the  $k$ -th iteration to obtain  $T_k(k,k) \neq 0$ .

(2.13) Example.

Compute EGP(A) where:

$$A = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 2 & 2 & 1 & 0 \\ -2 & -2 & 0 & -1 \\ -1 & -1 & 2 & -1 \end{bmatrix}$$

(\*)  $A_1 = A$ ;(\*)  $k = 1$ ;  $A_1(1,1) \neq 0 \Rightarrow P_1 = I$ ;  $T_1 = P_1 A_1$ ;

$$H_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \lambda_2 & 1 & 0 & 0 \\ \lambda_3 & 0 & 1 & 0 \\ \lambda_4 & 0 & 0 & 1 \end{bmatrix}$$

The values  $\lambda_2, \lambda_3, \lambda_4$  are determined by requiring that the elements (2,1), (3,1) and (4,1) - that is, the elements of the  $k$ -th column below the diagonal - in the matrix  $H_1 T_1$  be equal to zero:

$$\lambda_2 T_1(1,1) + T_1(2,1) = 0 \quad ; \quad \lambda_3 T_1(1,1) + T_1(3,1) = 0 \quad ; \quad \lambda_4 T_1(1,1) + T_1(4,1) = 0$$

Considering that  $T_1(1,1) \neq 0$ , the values  $\lambda_2, \lambda_3, \lambda_4$  are *uniquely determined*:

$$\lambda_2 = -\frac{T_1(2,1)}{T_1(1,1)} = -2 \quad ; \quad \lambda_3 = -\frac{T_1(3,1)}{T_1(1,1)} = 2 \quad ; \quad \lambda_4 = -\frac{T_1(4,1)}{T_1(1,1)} = 1$$

Finally:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 2 & 2 & 1 & 0 \\ -2 & 0 & 0 & -1 \\ -1 & 1 & 2 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 2 & -1 \end{bmatrix}$$

 $H_1$  $T_1$  $=$  $A_2$

(\*)  $k = 2$ ;  $A_2(2,2) = 0 \Rightarrow$  since it is *also*  $A_2(3,2) = A_2(4,2) = 0$ , the elements of the  $k$ -th column below the diagonal are *already equal to zero*, we set:  $P_2 = I$  and  $H_2 = I$ , from which  $T_2 = P_2 A_2 = A_2$  and  $A_3 = H_2 T_2 = H_2 A_2 = A_2$ ;

(\*)  $k = 3$ ;  $A_3(3,3) = 0 \Rightarrow$  since  $A_3(4,3) \neq 0$  we swap row three and four:  $P_3 = P_{3,4}$ , hence:

$$T_3 = P_3 A_3 = \begin{bmatrix} 1, & 1, & 0, & 0; \\ 0, & 0, & 1, & 0; \\ 0, & 0, & 2, & -1; \\ 0, & 0, & 0, & -1 \end{bmatrix}$$

This matrix is already upper triangular, so  $H_3 = I$  and  $A_4 = T_3$ ;

(\*)  $D = A_4$ ;  $P = P_3 P_2 P_1 = P_{3,4}$ ;

Then:

$$\begin{bmatrix} 1, & 0, & 0, & 0; \\ 2, & 1, & 0, & 0; \\ -2, & 0, & 1, & 0; \\ -1, & 0, & 0, & 1 \end{bmatrix} \begin{bmatrix} 1, & 0, & 0, & 0; \\ 0, & 1, & 0, & 0; \\ 0, & 0, & 0, & 1; \\ 0, & 0, & 1, & 0 \end{bmatrix} = \begin{bmatrix} 1, & 0, & 0, & 0; \\ 2, & 1, & 0, & 0; \\ -2, & 0, & 0, & 1; \\ -1, & 0, & 1, & 0 \end{bmatrix}$$

$$H_1^{-1} \quad P_{3,4}^t \quad \Sigma$$

and:

$$S = P \Sigma = \begin{bmatrix} 1, & 0, & 0, & 0; \\ 2, & 1, & 0, & 0; \\ -1, & 0, & 1, & 0; \\ -2, & 0, & 0, & 1 \end{bmatrix}$$

(2.14) Theorem (existence of LR factorization with pivoting).

Let  $A \in \mathbb{R}^{n \times n}$ . The EGP procedure applied to  $A$  returns a LR factorization of  $A$  with pivoting. That is: *for every*  $A \in \mathbb{R}^{n \times n}$  there exists *at least one* LR factorization with pivoting.

(Proof: It follows from the two previous examples.)

(2.15) Problem (use of the LR factorization with pivoting).

Let:

$$\text{EGP}(A) = \left( \begin{bmatrix} 1, & 0, & 0; \\ 0, & 1, & 0; \\ 1, & 1, & 1 \end{bmatrix}, \begin{bmatrix} 1, & 0, & 1; \\ 0, & 2, & 1; \\ 0, & 0, & -1 \end{bmatrix}, \begin{bmatrix} 0, & 1, & 0; \\ 1, & 0, & 0; \\ 0, & 0, & 1 \end{bmatrix} \right), \quad b = \begin{bmatrix} 1; \\ 0; \\ 0 \end{bmatrix}$$

*Without determining*  $A$ , decide whether  $A$  is invertible and, if so, determine the solution to the system  $A x = b$ .

(2.16) Procedure (study of a system of linear equations with EGP).

//  $A \in \mathbb{R}^{n \times n}$ ,  $b \in \mathbb{R}^n$ .

$(S,D,P) = \text{EGP}(A)$ ;

if there is  $k$  such that  $d_{kk} = 0$  then STOP; else  
 $c = SA(S, Pb);$   
 $x^* = SI(D, c)$

The procedure is *satisfactory* in the sense that, *however* given the data, it decides whether the matrix is invertible and, if so, determines the solution.

(2.17) Definition (the procedure GS).

A procedure for finding a QR factorization of a matrix  $A \in \mathbb{R}^{n \times n}$  is the following two-step one, called GS,<sup>1</sup> described in the special case of  $n = 3$ .

Let  $A = [a_1, a_2, a_3] \in \mathbb{R}^{3 \times 3}$ .

Step one.

We look for  $\Omega = [\omega_1, \omega_2, \omega_3]$  with orthogonal columns and  $\Theta$  with upper triangular form with  $\theta_{kk} = 1$  such that  $\Omega \Theta = A$ . *If such matrices exist*, rewriting the last equality column by column we get:

$$\omega_1 = a_1, \quad \omega_1 \theta_{1,2} + \omega_2 = a_2, \quad \omega_1 \theta_{1,3} + \omega_2 \theta_{2,3} + \omega_3 = a_3 \quad (*)$$

The first equality determines  $\omega_1$ . From the second it follows that:<sup>2</sup>

$$(\omega_1 \theta_{1,2}) \cdot \omega_1 + \omega_2 \cdot \omega_1 = a_2 \cdot \omega_1$$

Since  $\omega_1$  and  $\omega_2$  are orthogonal, we have  $\omega_2 \cdot \omega_1 = 0$ . Then, if  $\omega_1 \neq 0$ , we *necessarily* have:

$$\theta_{1,2} = (a_2 \cdot \omega_1) / (\omega_1 \cdot \omega_1)$$

hence:

$$\omega_2 = a_2 - \omega_1 \theta_{1,2}$$

From the third equality of (\*) we then have:

$$(\omega_1 \theta_{1,3}) \cdot \omega_1 + (\omega_2 \theta_{2,3}) \cdot \omega_1 + \omega_3 \cdot \omega_1 = a_3 \cdot \omega_1$$

and

$$(\omega_1 \theta_{1,3}) \cdot \omega_2 + (\omega_2 \theta_{2,3}) \cdot \omega_2 + \omega_3 \cdot \omega_2 = a_3 \cdot \omega_2$$

Since  $\omega_2 \cdot \omega_1 = 0$  and, analogously,  $\omega_3 \cdot \omega_1 = 0$ , then we *necessarily* have:

$$\theta_{1,3} = (a_3 \cdot \omega_1) / (\omega_1 \cdot \omega_1)$$

Since it is also  $\omega_3 \cdot \omega_2 = 0$ , if  $\omega_2 \neq 0$ , we *necessarily* have:

$$\theta_{2,3} = (a_3 \cdot \omega_2) / (\omega_2 \cdot \omega_2)$$

and, finally:

$$\omega_3 = a_3 - \omega_1 \theta_{1,3} - \omega_2 \theta_{2,3}$$

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1 The name GS of the procedure derives from that of the *Gram-Schmidt Orthonormalization Procedure*, from which it conceptually derives.

2 Given two columns  $v, w \in \mathbb{R}^n$ , we indicate with  $v \cdot w$  their canonical scalar product:  $v \cdot w = v_1 w_1 + \dots + v_n w_n$ .

Step two.

The factorization of  $A$  found in the previous step is *not* a QR factorization because the columns of  $\Omega$  do not have unit norm. This second step determines, if possible, a QR factorization by normalizing the columns of  $\Omega$ .

Let:  $\Delta = \text{diag}(\|\omega_1\|, \|\omega_2\|, \|\omega_3\|)$ .<sup>3</sup> If it is also  $\omega_3 \neq 0$ , the matrix  $\Delta$  it is invertible and it is easily verified that the couple

$$U = \Omega \Delta^{-1} \quad , \quad T = \Delta \Theta \quad (**) \quad$$

it is a QR factorization of  $A$ . Note that for the upper triangular matrix  $T$ , we have:

$$T_{k,k} = \|\omega_k\| > 0$$

(2.18) Theorem (procedure GS and QR factorization).

The GS Procedure described in the previous Definition determines a QR factorization of  $A \in \mathbb{R}^{n \times n}$  if and only if  $A$  is invertible.

(Proof. If the procedure does not terminate prematurely because  $\omega_k = 0$  for some  $k$ , then the pair  $U, T$  determined by  $(**)$  consists of two invertible matrices ( $U$  because it is orthogonal,  $T$  because it is triangular with the non-zero norms of the columns  $\omega_k$  on the diagonal). Conversely, if  $\omega_1 = 0$  then  $a_1 = 0$  and therefore  $A$  is not invertible. If  $\omega_1 \neq 0$  and  $\omega_2 = 0$  then  $0 = a_2 - \omega_1 \theta_{1,2} = a_2 - a_1 \theta_{1,2}$ , therefore  $a_1$  and  $a_2$  are linearly dependent, therefore  $A$  is not invertible. If  $\omega_1 \neq 0$ ,  $\omega_2 \neq 0$  and  $\omega_3 = 0 \dots$ )

(2.19) Remark (non-uniqueness of QR factorization).

Let  $A \in \mathbb{R}^{n \times n}$  and let  $U, T$  be a QR factorization of  $A$ . If  $E \in \mathbb{R}^{n \times n}$  is a diagonal matrix with, for example,  $E(1,1) = -1$  and  $E(k,k) = 1$  for  $k = 2, \dots, n$ , then the pair:

$$U' = U E \quad , \quad T' = E T$$

is a QR factorization of  $A$  *different* from  $U, T$ .

(2.20) Procedure (study of a system of linear equations with GS).

//  $A \in \mathbb{R}^{n \times n}$ ,  $b \in \mathbb{R}^n$ .

if GS( $A$ ) determines  $\omega_k = 0$  for some  $k$  then STOP; otherwise  
      $(U, T) = \text{GS}(A)$ ;  
      $x^* = \text{SI}(T, U^t b)$

This procedure is also *satisfactory* in the sense that, *however* given the data, it decides whether the matrix is invertible (using Theorem (2.18)) and, if so, determines the solution.

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3 Borrowing the symbology from *Scilab*,  $\text{diag}(v_1, \dots, v_n)$  indicates the diagonal matrix of size  $n \times n$  that has the elements  $v_1, \dots, v_n$  on the main diagonal.

(2.21) Remark (Householder method).

There are procedures that determine a QR factorization of *any*  $A \in \mathbb{R}^{n \times n}$  (even if non-invertible). For example, the following:

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(U,T) = Householder(A)

\\ A ∈ ℝn × n
A1 = A;
for k = 1,...,n-1 repeat:
    determine an orthogonal matrix  $X_k \in \mathbb{R}^{n \times n}$  such that the elements under the main
    diagonal of the first k columns of  $X_k A_k$  are zero and set:  $A_{k+1} = X_k A_k$ ;
T = An;
U = X1t ... Xn-1t
```

Scilab's qr function implements this procedure.

(2.22) Procedure ( study of a system of linear equations with Householder).

//  $A \in \mathbb{R}^{n \times n}$ ,  $b \in \mathbb{R}^n$ .

```
(U,T) = Householder(A);
if there is k such that  $t_{kk} = 0$  then STOP; otherwise  $x^* = SI(T, U^t b)$ 
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This procedure is also *satisfactory*.

## (2.1) CONDITIONING OF THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS

Let:

- $A \in \mathbb{R}^{n \times n}$  be an invertible matrix,  $b \in \mathbb{R}^n$  be a non-zero column and  $x^*$  be the solution of the system  $Ax = b$
- $A' \in \mathbb{R}^{n \times n}$  be an invertible matrix,  $b' \in \mathbb{R}^n$  be a column and  $\hat{x}$  be the solution of the system  $A'x = b'$

(2.23) Definition (data perturbations, deviation of the solution).

Let:

$$\delta A = A' - A \in \mathbb{R}^{n \times n}, \quad \delta b = b' - b \in \mathbb{R}^n$$

be the *data perturbations* and:

$$\delta x = \hat{x} - x^* \in \mathbb{R}^n$$

be the *deviation of the solution*.

(2.24) Problema (conditioning of the solution of a system of linear equations).

Given a way to *measure* data perturbations and the deviation of the solution, determine how

large the deviation of the solution *can be* as a function of how large the data perturbations *are*.