

# QR decomposition and Applications

**Recall:** The linear system of equations,

$$Ax = b, \text{ where } A \text{ is } n \times n \text{ and } b \in R^n,$$

can be solved using Gaussian elimination with partial pivoting. We have seen that this is equivalent to determining the permutation matrix  $P$  and lower and upper triangular matrices,  $L$  and  $U$  so that  $PA = LU$ . One then solves the system,  $Ax = b$ , by solving the equivalent system  $PAx = LUx = Pb$ . That is, we solve  $LUx = Pb$ , using standard forward substitution and back substitution (by first solving  $Lz = Pb$  and then solving  $Ux = z$ ).



# Error Analysis of GE

In exact arithmetic we have no truncation error in implementing GE and we would have  $LU = PA$ ,  $Lz = Pb$  and  $Ux = z$ .

When implemented in FP arithmetic we compute  $\bar{L}$ ,  $\bar{U}$ , and  $\bar{x}$ ,  $\bar{z}$ .

It can be shown that if GE is implemented in a FP system with  $n\mu < .01$ , then the computed  $\bar{x}$  of  $\bar{U}x = \bar{z}$  is the exact solution of,

$$(A + E)\bar{x} = b,$$

with  $E = (e_{i,j})$  satisfying

$$|e_{i,j}| < 1.02(2n^2 + n)\rho|A| \max_{i,j} |L_{i,j}|\mu,$$

where  $|A| = \max_{i,j} |a_{i,j}|$  and  $\rho$ , (the ‘growth factor’) is defined by

$$\rho = \frac{1}{|A|} \max_{i,j,r} |a_{i,j}^{(r)}|.$$



# Error Analysis of GE (Cont)

If ‘partial pivoting’ is used when implementing the  $LU$  decomposition, then one can show  $\max_{i,j} |L_{i,j}| = 1$  and  $\rho < 2^{n-1}$ .

- For a detailed, long but elementary proof of this result see Forsythe and Moler, *Computer Solution of Linear Equations*, Prentice Hall, pp. 87-108.
- The bound  $\rho < 2^{n-1}$  is pessimistic for most problems.
- With this strategy the corresponding error bound reduces to,

$$|e_{i,j}| \leq 1.02\rho|A|(2n^2 + n)\mu,$$

where  $\rho|A|$  can be monitored during the computation.

- The computed  $\bar{x}$  will “almost” satisfy the equation  $Ax = b$ , but what about  $|x - \bar{x}|$  ?



# A Simple Example

In a 4-digit, base 10, FP system consider,

$$.780x_1 + .563x_2 = .217$$

$$.913x_1 + .659x_2 = .254$$

The true solution is  $x = (1, -1)^T$ . Consider two approximate solutions obtained in FP arithmetic:  $\bar{x} = (.999, -1.001)^T$  and  $\hat{x} = (.341, -.087)^T$ . First determine the corresponding residuals,

$$\bar{r} \equiv A\bar{x} - b = (-.00136, -.00157)^T,$$

and

$$\hat{r} \equiv A\hat{x} - b = (-.000001, .000000)^T.$$

That is,  $\hat{x}$  is the exact solution of  $Ax = b + \hat{r}$ , where  $\|\hat{r}\| < 10^{-5}$ . This shows that a small residual does not imply a small error!



# Condition Number of $A$

To investigate  $\|x - \bar{x}\|$  we introduce matrix norms:

• For  $x \in \mathbb{R}^n$  consider two common vector norms,

$$\|x\|_{\infty} \equiv \max_{i=1}^n |x_i| \text{ and } \|x\|_2 \equiv (x^T x)^{1/2}.$$

• For  $A \in \mathbb{R}^{n \times n}$ ,  $A = (a_{i j})$ , we define the induced or subordinate matrix norm (corresponding to any vector norm) to be,

$$\|A\| \equiv \max_{\|v\|=1} \|Av\|.$$

For the above two examples:

$$\|A\|_{\infty} = \max_{i=1}^n \left[ \sum_{j=1}^n |a_{i j}| \right],$$

$$\begin{aligned} \|A\|_2^2 &= \max_{\|x\|_2=1} (Ax)^T (Ax) \\ &= \max_{\|x\|_2=1} [x^T (A^T A)x]. \end{aligned}$$



# Condition Number of $A$ (Cont)

Properties of matrix norms:

•  $\|AB\| \leq \|A\| \|B\|$  .

• If  $y = Ax$  we have  $\|y\| \leq \|A\| \|x\|$ .



# Recall – Property of GE

The computed  $\bar{x}$  determined by GE with partial pivoting has residual,  $\bar{r} \equiv A\bar{x} - b$  and satisfies, and

$$(A + E)\bar{x} = b \Rightarrow \bar{r} = A\bar{x} - b = -E\bar{x}.$$

From the properties of matrix norms,  $\|\bar{r}\|_\infty \leq \|E\|_\infty \|\bar{x}\|_\infty$ .

But  $E = (e_{ij})$  satisfies,

$$|e_{ij}| < 1.02\rho(2n^2 + n)|A|\mu,$$

and

$$\|\bar{r}\|_\infty \leq \|E\|_\infty \|\bar{x}\|_\infty \leq 1.02\rho(2n^3 + n^2)|A|\|\bar{x}\|_\infty\mu.$$

Therefore, GE with partial pivoting for any system  $Ax = b$  will generate an approximate solution,  $\bar{x}$  with a guaranteed small residual. In fact since  $|A|$ ,  $\|\bar{x}\|_\infty$ , and  $\rho$  are all known we have a precise bound on the size of the residual.



# What about $(\bar{x} - x)$ ?

The true solution  $x$  need not be close to  $\bar{x}$  since,

$$(\bar{x} - x) = \bar{x} - A^{-1}b = A^{-1}(A\bar{x} - b) = A^{-1}\bar{r},$$

and this implies

$$\begin{aligned}\|(\bar{x} - x)\|_{\infty} &\leq \|A^{-1}\|_{\infty}\|\bar{r}\|_{\infty} \\ &\leq \|A^{-1}\|_{\infty}\|A\|_{\infty}1.02\rho(2n^3 + n^2)\mu\|\bar{x}\|_{\infty}.\end{aligned}$$

Note:

- In general we do not know how large  $\|A^{-1}\|_{\infty}$  might be.
- If  $A$  is singular then  $A^{-1}$  is not defined so it is clear that if  $A$  is ‘nearly singular’ then  $\|A^{-1}\|_{\infty}$  must be very large.





# Condition Number

We define the Condition Number of  $A$ , wrt linear equations, to be.

$$\text{cond}(A) \equiv \|A\|_{\infty} \|A^{-1}\|_{\infty}.$$

Clearly  $\text{cond}(A)$  is an indication of how far away the computed  $\bar{x}$  might be from the true  $x$ .

When  $\text{cond}(A)$  is large the problem is said to be Ill-Conditioned since a small change in the RHS vector,  $b$ , can cause a large change in the solution vector,  $x$ . Consider the previous Example where we have,

$$A = \begin{bmatrix} .780 & .563 \\ .913 & .659 \end{bmatrix}, \quad A^{-1} = 10^6 \times \begin{bmatrix} .659 & -.563 \\ -.913 & .780 \end{bmatrix}.$$

In this case we have  $\text{cond}(A) = \|A\|_{\infty} \|A^{-1}\|_{\infty} = 2.6 \times 10^6$  which indicates an ill-conditioned problem.



# A Measure of Sensitivity

We have introduced the condition number to investigate the errors arising in GE with partial pivoting. It is actually a more general concept and can be defined for any matrix norm. In particular it describes the inherent sensitivity of the exact solution to small changes in the data defining the problem. To see this consider  $x$  to be the exact solution of  $Ax = b$  and  $x'$  the exact solution of  $Ax' = b + \epsilon$ . We then have,

$$x' = A^{-1}(b + \epsilon) = x + A^{-1}\epsilon = x + \delta,$$

where  $\|\delta\|_{\infty} = \|A^{-1}\epsilon\|_{\infty}$ . It is possible to choose the perturbation,  $\epsilon$  so that the resulting  $\delta$  satisfies

$$\|\delta\|_{\infty} = \|A^{-1}\|_{\infty}\|\epsilon\|_{\infty},$$

and we see how a small perturbation in  $b$  can result in a large change in the corresponding exact solution.



# QR Decomposition of A

An alternative to an LU decomposition.

A Householder Reflection is an elementary matrix of the form,

$$Q = I - 2ww^T,$$

where  $w \in \mathbb{R}^n$  satisfies  $\|w\|_2 = 1$ . (Recall that  $\|w\|_2 = 1 \Leftrightarrow w^T w = 1$ .) We will now investigate the use of HRs for solution of Linear Equations.

Properties of Householder reflections:

●  $Q^T = Q$  (symmetric) since

$$\begin{aligned} [I - 2ww^T]^T &= [I^T - 2(ww^T)^T] \\ &= [I - 2(w^T)^T w^T] \\ &= [I - 2ww^T] \\ &= Q \end{aligned}$$



# Properties of HRs (cont.)

•  $Q^T Q = Q^2 = I$  since ,

$$\begin{aligned}[I - 2ww^T][I - 2ww^T] &= I - 4ww^T + 4ww^T ww^T \\ &= I - 4ww^T + 4w(w^T w)w^T \\ &= I - 4ww^T + 4ww^T \\ &= I.\end{aligned}$$

Therefore we have  $Q^{-1} = Q = Q^T$ .

•  $\|Q\|_2 = 1$ , since for a general matrix  $A$  we have,

$$\|A\|_2^2 = \max_{\|x\|_2=1} \{x^T (A^T A)x\},$$

and therefore, for a Householder reflection,

$$\|Q\|_2^2 = \max_{\|x\|_2=1} \{x^T (Q^T Q)x\} = \max_{\|x\|_2=1} \{x^T x\} = 1.$$



# Properties of HRs (cont.)

• if  $y = Qx$  then  $\|y\|_2 = \|x\|_2$  since,

$$\|y\|_2^2 = y^T y = (Qx)^T Qx = x^T (Q^T Q)x = x^T x = \|x\|_2^2.$$

We usually define  $Q$  in terms of an arbitrary vector  $u \in \mathbb{R}^n$  by,

$$Q = \left[ I - 2 \frac{uu^T}{\|u\|_2^2} \right],$$

Note that this corresponds to  $w = u/\|u\|_2$  but it avoids computing a square root and the normalization of  $u$ .



# The Choice of $u$ to define $Q$

Consider the affect of a Householder reflection applied to a vector  $x$ ,  $y = Qx$ ,

$$y = \left[ I - 2 \frac{uu^T}{\|u\|_2^2} \right] x = x - 2 \frac{u^T x}{\|u\|_2^2} u = x + \gamma u.$$

That is,  $u = (y - x)/\gamma$  or  $u$  is a multiple of  $(y - x)$ . This implies that for any  $y$  such that  $\|y\|_2 = \|x\|_2$  we can map  $x$  onto  $y$  using

$$Q = \left[ I - 2 \frac{(y - x)(y - x)^T}{\|y - x\|_2^2} \right].$$



# An Example of a HR

Determine the value(s) of  $t \in \mathfrak{R}$  such that there exists a Householder reflection,  $Q$  that maps  $x = (7, 0, 1)^T$  onto  $y = (0, 5, t)^T$  and find the corresponding transformation(s). To do this we first observe that since the 2-norm must be preserved, we must have  $7^2 + 1^2 = 5^2 + t^2$  or  $t = \pm 5$ . Consider the solution corresponding to  $t = -5$ ,

$$u = y - x = \begin{bmatrix} 0 \\ 5 \\ -5 \end{bmatrix} - \begin{bmatrix} 7 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -7 \\ 5 \\ -6 \end{bmatrix}.$$

We then have  $\|u\|_2^2 = 110$  and  $-2/\|u\|_2^2 = (-1/55)$ .



# An Example of a HR (cont.)

The corresponding  $Q = I - 2\frac{uu^T}{\|u\|_2^2}$ , is then,

$$Q = I - \frac{1}{55} \begin{bmatrix} 49 & -35 & 42 \\ -35 & 25 & -30 \\ 42 & -30 & 36 \end{bmatrix} \\ = \begin{bmatrix} 6/55 & 35/55 & -42/55 \\ 35/55 & 30/55 & 30/55 \\ -42/55 & 30/55 & 19/55 \end{bmatrix}.$$

Exercise. Determine the corresponding  $Q$  for  $t = 5$ .





# Factoring $A$ using HRs

A Householder reflection can be used to transform a given vector  $x = [x_1, x_2 \cdots x_r \cdots x_n]^T$  onto  $[x_1, x_2 \cdots x_{r-1}, s, 0, 0 \cdots 0]^T = y^T$  where,

$$s^2 = x_r^2 + x_{r+1}^2 \cdots x_n^2.$$

The corresponding  $u$  satisfies,

$$u = y - x = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ -x_r \pm s \\ -x_{r+1} \\ \vdots \\ -x_n \end{bmatrix},$$

where the sign of  $s$  is usually chosen to agree with the sign of  $-x_r$  (no loss of significance).



# Efficient Computation of $Qv$

With this choice of  $u$ ,

$$Qv = \left[ I - 2 \frac{uu^T}{\|u\|_2^2} \right] v = v - \left( \frac{2u^T v}{\|u\|_2^2} \right) u.$$

That is, we form the scalar  $u^T v$  and then add a multiple of  $u$  to  $v$ . This transformation will leave the first  $(r - 1)$  entries of  $v$  unchanged. It also has no effect on  $v$  if  $u^T v = 0$  (in particular, if  $v_{r+1} = v_{r+2} = \dots = v_n = 0$ ).



# Factoring $A = QR$

Now consider factoring  $A = QR$  (rather than  $A = LU$ ), where  $R$  is upper triangular and  $Q = Q_1 Q_2 \cdots Q_{n-1}$ , a product of Householder reflections. Note that,

$$Q^{-1} = Q^T = Q_{n-1}^T Q_{n-2}^T \cdots Q_1^T = Q_{n-1} Q_{n-2} \cdots Q_1 \neq Q.$$

This factoring (or decomposition of  $A$ ) is accomplished (analogous to  $LU$ ) by first setting  $A_0 = A$  and choosing  $Q_1$  to introduce zeros below the diagonal of the first column of  $A_1 = Q_1 A_0$ ,

$$A_1 = \begin{bmatrix} s_1 & & & & \\ 0 & & & & \\ 0 & (Q_1 \underline{a}_2^{(0)}) & \cdots & (Q_1 \underline{a}_n^{(0)}) & \\ \vdots & & & & \\ 0 & & & & \end{bmatrix}.$$



# First Step of $QR$ Decomp of $A$

From above we see that this can be done with  $Q_1$  defined by  $u_1$ ,

$$u_1 = \begin{bmatrix} -a_{1\ 1}^{(0)} \pm s_1 \\ -a_{2\ 1}^{(0)} \\ \vdots \\ -a_{n\ 1}^{(0)} \end{bmatrix},$$

where  $s_1^2 = (a_{1\ 1}^{(0)})^2 + (a_{2\ 1}^{(0)})^2 \cdots (a_{n\ 1}^{(0)})^2$ . In general at the  $r^{th}$  stage,

$$A_{r-1} = \begin{bmatrix} a_{1\ 1}^{(r-1)} & a_{1\ 2}^{(r-1)} & \cdots & a_{1\ r}^{(r-1)} & \cdots & a_{1\ n}^{(r-1)} \\ 0 & a_{2\ 2}^{(r-1)} & \cdots & a_{2\ r}^{(r-1)} & \cdots & a_{2\ n}^{(r-1)} \\ 0 & 0 & \cdots & a_{3\ r}^{(r-1)} & \cdots & a_{3\ n}^{(r-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{r\ r}^{(r-1)} & \cdots & a_{r\ n}^{(r-1)} \\ 0 & 0 & \cdots & a_{r+1\ r}^{(r-1)} & \cdots & a_{r+1\ n}^{(r-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{n\ r}^{(r-1)} & \cdots & a_{n\ n}^{(r-1)} \end{bmatrix}.$$



# $r^{\text{th}}$ Step of $QR$ Decomp of $A$

We choose  $Q_r$  to map

$$\underline{a}_r^{(r-1)} \rightarrow (a_{1r}^{(r-1)}, a_{2r}^{(r-1)} \cdots a_{r-1r}^{(r-1)}, s_r, 0 \cdots 0)^T,$$

$$s_r^2 = (a_{1r}^{(r-1)})^2 + (a_{2r}^{(r-1)})^2 \cdots + (a_{nr}^{(r-1)})^2.$$

That is,

$$u_r = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ -a_{1r}^{(r-1)} \pm s_r \\ -a_{2r}^{(r-1)} \\ \vdots \\ -a_{nr}^{(r-1)} \end{bmatrix}.$$



$$Q^T A = R$$

As with the  $LU$  factorization of  $A$  we have, after  $(n - 1)$  steps,

$$\begin{aligned} Q^T A &= Q^T A_0 \\ &= [Q_1 Q_2 \cdots Q_{n-1}]^T A_0 \\ &= [Q_{n-1} Q_{n-2} \cdots Q_1] A_0 \\ &= (Q_{n-1} (\cdots (Q_2 (\underbrace{Q_1 A_0}_{A_1}))) \cdots) \\ &= A_{n-1} \\ &\equiv R \end{aligned}$$

Since  $Q^T A = R$  and  $Q^T = Q^{-1}$  we have, after multiplying this expression by  $Q$ ,

$$QR = Q(Q^T A) = (QQ^T)A = A.$$

**Exercise:** Show that the operation count for this decomposition is twice that for the  $LU$  decomposition.

