

## Applied Numerical Linear Algebra. Lecture 8

# Householder Transformations

A Householder transformation (or reflection) is a matrix of the form  $P = I - 2uu^T$  where  $\|u\|_2 = 1$ . It is easy to see that  $P = P^T$  and  $P \cdot P^T = (I - 2uu^T)(I - 2uu^T) = I - 4uu^T + 4uu^T uu^T = I$ , so  $P$  is a symmetric, orthogonal matrix. It is called a reflection because  $Px$  is reflection of  $x$  in the plane through 0 perpendicular to  $u$ .

Given a vector  $x$ , it is easy to find a Householder reflection  $P = I - 2uu^T$  to zero out all but the first entry of  $x$ :  $Px = [c, 0, \dots, 0]^T = c \cdot e_1$ . We do this as follows. Write  $Px = (I - 2uu^T)x = x - 2u(u^T x) = c \cdot e_1$  so from that equation we get  $u = \frac{1}{2(u^T x)}(x - ce_1)$ , i.e.,  $u$  is a linear combination of  $x$  and  $e_1$ . Since  $\|x\|_2 = \|Px\|_2 = |c|$ ,  $u$  must be parallel to the vector  $\tilde{u} = x \pm \|x\|_2 e_1$ , and so  $u = \tilde{u} / \|\tilde{u}\|_2$ . One can verify that either choice of sign yields a  $u$  satisfying  $Px = ce_1$ , as long as  $\tilde{u} \neq 0$ . We will use  $\tilde{u} = x + \text{sign}(x_1)e_1$ , since this means that there is no cancellation in computing the first component of  $u$ . Here,  $x_k$  is to be the pivot coordinate in the vector  $x$  after which all entries are 0 in matrix  $A$ . In summary, we get

$$\tilde{u} = \begin{bmatrix} x_1 + \text{sign}(x_1) \cdot \|x\|_2 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \text{with } u = \frac{\tilde{u}}{\|\tilde{u}\|_2}.$$

We write this as  $u = \text{House}(x)$ . (In practice, we can store  $\tilde{u}$  instead of  $u$  to save the work of computing  $u$ , and use the formula  $P = I - (2/\|\tilde{u}\|_2^2)\tilde{u}\tilde{u}^T$  instead of  $P = I - 2uu^T$ .)

# Idea of Householder transformation

We show how to compute the QR decomposition of a 5-by-4 matrix  $A$  using Householder transformations. This example will make the pattern for general  $m$ -by- $n$  matrices evident. In the matrices below,  $P_i$  is an orthogonal matrix,  $x$  denotes a generic nonzero entry, and  $o$  denotes a zero entry.

1. Choose  $P_1$  so

$$A_1 \equiv P_1 A = \begin{bmatrix} x & x & x & x \\ o & x & x & x \\ o & x & x & x \\ o & x & x & x \\ o & x & x & x \end{bmatrix}.$$

2. Choose  $P_2 = \left[ \begin{array}{c|c} 1 & 0 \\ \hline 0 & P'_2 \end{array} \right]$  so

$$A_2 \equiv P_2 A_1 = \begin{bmatrix} x & x & x & x \\ o & x & x & x \\ o & o & x & x \\ o & o & x & x \\ o & o & x & x \end{bmatrix}.$$

3. Choose  $P_3 = \left[ \begin{array}{ccc|c} 1 & & & 0 \\ & & & \\ & & 1 & \\ \hline & 0 & & P'_3 \end{array} \right]$  so

$$A_3 \equiv P_3 A_2 = \begin{bmatrix} x & x & x & x \\ o & x & x & x \\ o & o & x & x \\ o & o & o & x \\ o & o & o & x \end{bmatrix}.$$

4. Choose  $P_4 = \left[ \begin{array}{ccc|c} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ \hline & 0 & & P'_4 \end{array} \right]$  so

$$\tilde{R} := A_4 \equiv P_4 A_3 = \begin{bmatrix} x & x & x & x \\ o & x & x & x \\ o & o & x & x \\ o & o & o & x \\ o & o & o & o \end{bmatrix}.$$

Here, we have chosen a Householder matrix  $P'_i$  to zero out the subdiagonal entries in column  $i$ ; this does not disturb the zeros already introduced in previous columns.

# Idea of Householder transformation

We observe that we have performed decomposition

$$A_4 = P_4 P_3 P_2 P_1 A. \quad (1)$$

Let us denote the final triangular matrix  $A_4$  as  $\tilde{R} \equiv A_4$ . Then using (1) we observe that matrix  $A$  is obtained via decomposition

$$A = P_1^T P_2^T P_3^T P_4^T \tilde{R} = QR, \quad (2)$$

which is our desired QR decomposition. Here, the matrix  $Q$  is the first four columns of  $P_1^T P_2^T P_3^T P_4^T = P_1 P_2 P_3 P_4$  (since all  $P_i$  are symmetric), and  $R$  is the first four rows of  $\tilde{R}$ .

◇

Here is the general algorithm for QR decomposition using Householder transformations.

ALGORITHM 3.2. *QR factorization using Householder reflections:*

```
for  $i = 1$  to  $\min(m - 1, n)$ 
     $u_i = \text{House}(A(i : m, i))$ 
     $P'_i = I - 2u_i u_i^T$ 
     $A(i : m, i : n) = P'_i A(i : m, i : n)$ 
end for
```



# QR decomposition using Householder reflections

We can use Householder reflections to calculate the QR factorization of an  $m$ -by- $n$  matrix  $A$  with  $m \geq n$ .

- Let  $\mathbf{x}$  be an arbitrary real  $m$ -dimensional column vector of  $A$  such that  $\|\mathbf{x}\| = |\alpha|$  for a scalar  $\alpha$ .
- If the algorithm is implemented using floating-point arithmetic, then  $\alpha$  should get the opposite sign as the  $k$ -th coordinate of  $\mathbf{x}$ , where  $x_k$  is to be the pivot coordinate after which all entries are 0 in matrix  $A$ 's final upper triangular form, to avoid loss of significance.

Then, where  $\mathbf{e}_1$  is the vector  $(1, 0, \dots, 0)^T$ ,  $\|\cdot\|$  is the Euclidean norm and  $I$  is an  $m$ -by- $m$  identity matrix, set

$$\mathbf{v} = \mathbf{x} + \alpha \mathbf{e}_1,$$

$$\alpha = -\text{sign}(x_1) \|\mathbf{x}\|,$$

$$\mathbf{u} = \frac{\mathbf{v}}{\|\mathbf{v}\|},$$

$$Q = I - 2\mathbf{u}\mathbf{u}^T.$$

In the case of complex  $A$  set

$$Q = I - (1 + w)\mathbf{u}\mathbf{u}^H,$$

where  $w = \mathbf{x}^H \mathbf{u} / \mathbf{u}^H \mathbf{x}$  and where  $\mathbf{x}^H$  is the conjugate transpose (transjugate) of  $\mathbf{x}$ ,

$Q$  is an  $m$ -by- $m$  Householder matrix and

$$Q\mathbf{x} = (\alpha, 0, \dots, 0)^T.$$

This can be used to gradually transform an  $m$ -by- $n$  matrix  $A$  to upper triangular form. First, we multiply  $A$  with the Householder matrix  $Q_1$  we obtain when we choose the first matrix column for  $x$ . This results in a matrix  $Q_1A$  with zeros in the left column (except for the first row).

$$Q_1A = \begin{bmatrix} \alpha_1 & * & \dots & * \\ 0 & & & \\ \vdots & & A' & \\ 0 & & & \end{bmatrix}$$

This can be repeated for  $A'$  (obtained from  $Q_1A$  by deleting the first row and first column), resulting in a Householder matrix  $Q'_2$ . Note that  $Q'_2$  is smaller than  $Q_1$ . Since we want it really to operate on  $Q_1A$  instead of  $A'$  we need to expand it to the upper left, filling in  $a_1$ , or in general:

$$Q_k = \begin{pmatrix} I_{k-1} & 0 \\ 0 & Q'_k \end{pmatrix}.$$

After  $t$  iterations of this process,  $t = \min(m - 1, n)$ ,

$$R = Q_t \cdots Q_2 Q_1 A$$

is an upper triangular matrix. So, with

$$Q = Q_1^T Q_2^T \cdots Q_t^T,$$

$A = QR$  is a  $QR$  decomposition of  $A$ .

# Example how to compute QR decomposition using Householder reflections.

Let us calculate the decomposition of

$$A = \begin{pmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{pmatrix}.$$

First, we need to find a reflection that transforms the first column of matrix  $A$ , vector  $\mathbf{x} = \mathbf{a}_1 = (12, 6, -4)^T$ , to

$$\|\mathbf{x}\| \mathbf{e}_1 = \|\mathbf{a}_1\| \mathbf{e}_1 = (14, 0, 0)^T.$$

Now,

$$\mathbf{v} = \mathbf{x} + \alpha \mathbf{e}_1,$$

where

$$\alpha = -\text{sign}(x_1) \|\mathbf{x}\|,$$

and

$$\mathbf{u} = \frac{\mathbf{v}}{\|\mathbf{v}\|}.$$

Here,  $\|\mathbf{x}\| = \sqrt{12^2 + 6^2 + (-4)^2} = 14$ ,

$$\alpha = -\text{sign}(12)\|\mathbf{x}\| = -14 \text{ and } \mathbf{x} = \mathbf{a}_1 = (12, 6, -4)^T$$

Therefore

$$\mathbf{v} = \mathbf{x} + \alpha \mathbf{e}_1 = (-2, 6, -4)^T = (2)(-1, 3, -2)^T$$

and  $\mathbf{u} = \frac{\mathbf{v}}{\|\mathbf{v}\|} = \frac{1}{\sqrt{14}}(-1, 3, -2)^T$ , and then

$$\begin{aligned} Q_1 &= I - \frac{2}{\sqrt{14}\sqrt{14}} \begin{pmatrix} -1 \\ 3 \\ -2 \end{pmatrix} \begin{pmatrix} -1 & 3 & -2 \end{pmatrix} \\ &= I - \frac{1}{7} \begin{pmatrix} 1 & -3 & 2 \\ -3 & 9 & -6 \\ 2 & -6 & 4 \end{pmatrix} \\ &= \begin{pmatrix} 6/7 & 3/7 & -2/7 \\ 3/7 & -2/7 & 6/7 \\ -2/7 & 6/7 & 3/7 \end{pmatrix}. \end{aligned}$$

Now observe:

$$A_1 = Q_1 A = \begin{pmatrix} 14 & 21 & -14 \\ 0 & -49 & -14 \\ 0 & 168 & -77 \end{pmatrix},$$

so we already have almost a triangular matrix. We only need to zero the (3, 2) entry.

Take the (1, 1) minor, and then apply the process again to

$$A' = M_{11} = \begin{pmatrix} -49 & -14 \\ 168 & -77 \end{pmatrix}.$$

By the same method as above we first need to find a reflection that transforms the first column of matrix  $A'$ , vector  $\mathbf{x} = (-49, 168)^T$ , to  $\|\mathbf{x}\| \mathbf{e}_1 = (175, 0)^T$ . Here,  $\|\mathbf{x}\| = \sqrt{(-49)^2 + 168^2} = 175$ ,

$$\alpha = -\text{sign}(-49)\|\mathbf{x}\| = 175 \text{ and } \mathbf{x} = (-49, 168)^T.$$

Therefore

$$\mathbf{v} = \mathbf{x} + \alpha \mathbf{e}_1 = (-49, 168)^T + (175, 0)^T = (126, 168)^T,$$

$$\|\mathbf{v}\| = \sqrt{126^2 + 168^2} = \sqrt{44100} = 210 \text{ and}$$

$$\mathbf{u} = \frac{\mathbf{v}}{\|\mathbf{v}\|} = (126/210, 168/210)^T = (3/5, 4/5)^T.$$

Then

$$Q'_2 = I - 2 \begin{pmatrix} 3/5 \\ 4/5 \end{pmatrix} \begin{pmatrix} 3/5 & 4/5 \end{pmatrix}$$

or

$$\begin{aligned} Q'_2 &= I - 2 \begin{pmatrix} 9/25 & 12/25 \\ 12/25 & 16/25 \end{pmatrix} \\ &= \begin{pmatrix} 7/25 & -24/25 \\ -24/25 & -7/25 \end{pmatrix} \end{aligned}$$

Finally, we obtain the matrix of the Householder transformation  $Q_2$  such that

$$Q_2 = \left[ \begin{array}{c|c} 1 & 0 \\ \hline 0 & Q'_2 \end{array} \right]$$

to get

$$Q_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 7/25 & -24/25 \\ 0 & -24/25 & -7/25 \end{pmatrix}$$

after performing a direct sum with 1 to make sure the next step in the process works properly.



Now, we find

$$Q = Q_1^T Q_2^T = \begin{pmatrix} 6/7 & 69/175 & -58/175 \\ 3/7 & -158/175 & 6/175 \\ -2/7 & -6/35 & -33/35 \end{pmatrix}$$

Then

$$Q = Q_1^T Q_2^T = \begin{pmatrix} 0.8571 & 0.3943 & -0.3314 \\ 0.4286 & -0.9029 & 0.0343 \\ -0.2857 & -0.1714 & -0.9429 \end{pmatrix}$$

$$R = Q_2 A_1 = Q_2 Q_1 A = Q^T A = \begin{pmatrix} 14 & 21 & -14 \\ 0 & -175 & 70 \\ 0 & 0 & 35 \end{pmatrix}.$$

The matrix  $Q$  is orthogonal and  $R$  is upper triangular, so  $A = QR$  is the required QR-decomposition.

Note:

$$\begin{aligned} Q_2 Q_1 A &= R, \\ Q_1^T Q_2^T Q_2 Q_1 A &= Q_1^T Q_2^T R \\ A &= Q_1^T Q_2^T R = QR, \\ \text{with } Q &= Q_1^T Q_2^T. \end{aligned}$$

## Example

Compute  $QR$  decomposition of the matrix  $A$  using Householder reflections:

$$\mathbf{A} = \begin{bmatrix} 4 & 4 & 3 \\ 0 & 3 & 1 \\ 3 & 4 & 7 \end{bmatrix}$$

First, we need to find a reflection that transforms the first column of matrix  $A$

$$\mathbf{A} = \begin{bmatrix} 4 & 4 & 3 \\ 0 & 3 & 1 \\ 3 & 4 & 7 \end{bmatrix}$$

We have:

$$\mathbf{u} = \mathbf{x} + \alpha \mathbf{e}_1,$$

where  $\mathbf{x} = (4, 0, 3)^T$ ,  $\alpha = -\text{sign}(4) \cdot \|\mathbf{x}\|$

$$\mathbf{v} = \frac{\mathbf{u}}{\|\mathbf{u}\|}.$$

Here,

$$\alpha = -5.$$

Therefore

$$\mathbf{u} = (-1, 0, 3)^T, \quad \|\mathbf{u}\| = \sqrt{10}.$$

and  $\mathbf{v} = \frac{1}{\sqrt{10}}(-1, 0, 3)^T$ , and then

$$\begin{aligned} P_1 &= I - \frac{2}{\sqrt{10}\sqrt{10}} \begin{pmatrix} -1 \\ 0 \\ 3 \end{pmatrix} (-1 \ 0 \ 3) \\ &= I - \frac{1}{5} \begin{pmatrix} 1 & 0 & -3 \\ 0 & 0 & 0 \\ -3 & 0 & 9 \end{pmatrix} \\ &= \begin{pmatrix} 4/5 & 0 & 3/5 \\ 0 & 1 & 0 \\ 3/5 & 0 & -4/5 \end{pmatrix}. \end{aligned}$$

Now observe:

$$P_1 A = \begin{pmatrix} 5 & 5.6 & 6.6 \\ 0 & 3 & 1 \\ 0 & -0.8 & -3.8 \end{pmatrix},$$

so we already have almost a triangular matrix. We only need to zero the (3, 2) entry.

Take the (1,1) minor, and then apply the process again to

$$A' = M_{11} = \begin{pmatrix} 3 & 1 \\ -0.8 & -3.8 \end{pmatrix}.$$

We have:

$$\mathbf{u} = \mathbf{x} + \alpha \mathbf{e}_1,$$

where  $\mathbf{x} = (3, -0.8)^T$ ,  $\alpha = -\text{sign}(3) \cdot \|\mathbf{x}\|$

$$\mathbf{v} = \frac{\mathbf{u}}{\|\mathbf{u}\|}.$$

Here,

$$\alpha = -3.1048.$$

Therefore

$$\mathbf{u} = (-0.1048, -0.8)^T, \quad \|\mathbf{u}\| = 0.8068.$$

and  $\mathbf{v} = \frac{1}{0.8068}(-0.1048, -0.8)^T$ ,

and then

$$\begin{aligned}P_2' &= I - \frac{2}{0.651} \begin{pmatrix} -0.1048 \\ -0.8 \end{pmatrix} \begin{pmatrix} -0.1048 & -0.8 \end{pmatrix} \\ &= I - \frac{2}{0.651} \begin{pmatrix} 0.011 & 0.0838 \\ 0.0838 & 0.64 \end{pmatrix} \\ &= \begin{pmatrix} 0.9662 & -0.2575 \\ 0.2575 & -0.9662 \end{pmatrix}.\end{aligned}$$

Then the second matrix of the Householder transformation is

$$P_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0.9662 & -0.2575 \\ 0 & -0.2575 & -0.9662 \end{pmatrix}$$

Now, we find

$$R = P_2 P_1 A = \begin{pmatrix} 5 & 5.6 & 6.6 \\ 0 & 3.1046 & 1.9447 \\ 0 & 0.0005 & 3.4141 \end{pmatrix}.$$

The matrix  $P$  is orthogonal and  $R$  is upper triangular, so  $A = QR$  is the required QR-decomposition with  $P = P_1^T P_2^T$ .

# Tridiagonalization using Householder transformation

This procedure is taken from the book: Numerical Analysis, Burden and Faires, 8th Edition.

In the first step, to form the Householder matrix in each step we need to determine  $\alpha$  and  $r$ , which are given by:

$$\alpha = -\text{sgn}(a_{21}) \sqrt{\sum_{j=2}^n a_{j1}^2};$$

$$r = \sqrt{\frac{1}{2}(\alpha^2 - a_{21}\alpha)};$$

From  $\alpha$  and  $r$ , construct vector  $v$ :

$$v^{(1)} = \begin{bmatrix} v_1 \\ v_2 \\ \dots \\ v_n \end{bmatrix},$$

where  $v_1 = 0$ ;  $v_2 = \frac{a_{21} - \alpha}{2r}$ , and

$$v_k = \frac{a_{k1}}{2r} \text{ for each } k = 3, 4..n$$

Then compute:

$$P^1 = I - 2v^{(1)}(v^{(1)})^t$$

and obtaining matrix  $A^{(1)}$  as

$$A^{(1)} = P^1 A P^1$$



Having found  $P^{(1)}$  and computed  $A^{(1)}$  the process is repeated for  $k = 2, 3, \dots, n$  as follows:

$$\alpha = -\operatorname{sgn}(a_{k+1,k}) \sqrt{\sum_{j=k+1}^n a_{jk}^2};$$

$$r = \sqrt{\frac{1}{2}(\alpha^2 - a_{k+1,k}\alpha)};$$

$$v_1^{(k)} = v_2^{(k)} = \dots = v_k^{(k)} = 0;$$

$$v_{k+1}^{(k)} = \frac{a_{k+1,k} - \alpha}{2r}$$

$$v_j^{(k)} = \frac{a_{jk}}{2r} \quad \text{for } j = k+2; k+3, \dots, n$$

$$P^k = I - 2v^{(k)}(v^{(k)})^T$$

$$A^{(k+1)} = P^k A^{(k)} P^k$$

# Example 1

In this example, the given matrix  $A$  is transformed to the similar tridiagonal matrix  $A_1$  by using Householder Method. We have

$$\mathbf{A} = \begin{bmatrix} 5 & 1 & 0 \\ 1 & 6 & 3 \\ 0 & 3 & 7 \end{bmatrix},$$

Steps:

1. First compute  $\alpha$  as

$$\alpha = -\operatorname{sgn}(a_{21}) \sqrt{\sum_{j=2}^n a_{j1}^2} = -\sqrt{(a_{21}^2 + a_{31}^2)} = -\sqrt{(1^2 + 0^2)} = -1.$$

2. Using  $\alpha$  we find  $r$  as

$$r = \sqrt{\frac{1}{2}(\alpha^2 - a_{21}\alpha)} = \sqrt{\frac{1}{2}((-1)^2 - 1 \cdot (-1))} = 1.$$

3. From  $\alpha$  and  $r$ , construct vector  $v$ :

$$v^{(1)} = \begin{bmatrix} v_1 \\ v_2 \\ \dots \\ v_n \end{bmatrix},$$

where  $v_1 = 0$ ;  $v_2 = \frac{a_{21}-\alpha}{2r}$ , and

$$v_k = \frac{a_{k1}}{2r} \text{ for each } k = 3, 4..n$$

To do that we compute:

$$\begin{aligned}v_1 &= 0, \\v_2 &= \frac{a_{21} - \alpha}{2r} = \frac{1 - (-1)}{2 \cdot 1} = 1, \\v_3 &= \frac{a_{31}}{2r} = 0.\end{aligned}$$

and we have

$$v^{(1)} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},$$

Then compute matrix  $P^{(1)}$

$$P^{(1)} = I - 2v^{(1)}(v^{(1)})^T$$

and

$$P^{(1)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

After that we can obtain matrix  $A^{(1)}$  as

$$A^{(1)} = P^{(1)}AP^{(1)} = \begin{bmatrix} 5 & -1 & 0 \\ -1 & 6 & -3 \\ 0 & -3 & 7 \end{bmatrix}$$

## Example 2

In this example, the given matrix  $A$  is transformed to the similar tridiagonal matrix  $A_2$  by using Householder Method. We have

$$\mathbf{A} = \begin{bmatrix} 4 & 1 & -2 & 2 \\ 1 & 2 & 0 & 1 \\ -2 & 0 & 3 & -2 \\ 2 & 1 & -2 & -1 \end{bmatrix},$$

Steps:

1. First compute  $\alpha$  as

$$\begin{aligned}\alpha &= -\operatorname{sgn}(a_{21}) \sqrt{\sum_{j=2}^n a_{j1}^2} = (-1) \cdot \sqrt{(a_{21}^2 + a_{31}^2 + a_{41}^2)} \\ &= -1 \cdot (1^2 + (-2)^2 + 2^2) = (-1) \cdot \sqrt{1 + 4 + 4} = -\sqrt{9} = -3.\end{aligned}$$

2. Using  $\alpha$  we find  $r$  as

$$r = \sqrt{\frac{1}{2}(\alpha^2 - a_{21}\alpha)} = \sqrt{\frac{1}{2}((-3)^2 - 1 \cdot (-3))} = \sqrt{6}.$$



3. From  $\alpha$  and  $r$ , construct vector  $v$ :

$$v^{(1)} = \begin{bmatrix} v_1 \\ v_2 \\ \dots \\ v_n \end{bmatrix},$$

where  $v_1 = 0$ ;  $v_2 = \frac{a_{21} - \alpha}{2r}$ , and

$$v_k = \frac{a_{k1}}{2r} \text{ for each } k = 3, 4..n$$

To do that we compute:

$$v_1 = 0,$$

$$v_2 = \frac{a_{21} - \alpha}{2r} = \frac{1 - (-3)}{2 \cdot \sqrt{6}} = \frac{2}{\sqrt{6}}$$

$$v_3 = \frac{a_{31}}{2r} = \frac{-2}{2 \cdot \sqrt{6}} = \frac{-1}{\sqrt{6}}$$

$$v_4 = \frac{a_{41}}{2r} = \frac{2}{2 \cdot \sqrt{6}} = \frac{1}{\sqrt{6}}.$$

and we have

$$v^{(1)} = \begin{bmatrix} 0 \\ \frac{2}{\sqrt{6}} \\ \frac{-1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{bmatrix},$$

Then compute matrix  $P^{(1)}$

$$P^{(1)} = I - 2v^{(1)}(v^{(1)})^T = I - 2 \cdot \begin{bmatrix} 0 \\ \frac{2}{\sqrt{6}} \\ \frac{-1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{bmatrix} \cdot \begin{bmatrix} 0 & \frac{2}{\sqrt{6}} & \frac{-1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{bmatrix}$$

and

$$P^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1/3 & 2/3 & -2/3 \\ 0 & 2/3 & 2/3 & 1/3 \\ 0 & -2/3 & 1/3 & 2/3 \end{bmatrix}$$

After that we can obtain matrix  $A^{(1)}$  as

$$A^{(1)} = P^{(1)}AP^{(1)}$$

Thus, the first Householder matrix:

$$P^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1/3 & 2/3 & -2/3 \\ 0 & 2/3 & 2/3 & 1/3 \\ 0 & -2/3 & 1/3 & 2/3 \end{bmatrix},$$

$$A^{(1)} = P^{(1)}AP^{(1)} = \begin{bmatrix} 4 & -3 & 0 & 0 \\ -3 & 10/3 & 1 & 4/3 \\ 0 & 1 & 5/3 & -4/3 \\ 0 & 4/3 & -4/3 & -1 \end{bmatrix},$$

Next, having found  $A^{(1)}$  we need to construct  $A^{(2)}$  and  $P^{(2)}$ . When  $k = 2$  we have following formulas:

$$\alpha = -\operatorname{sgn}(a_{3,2}) \sqrt{\sum_{j=3}^4 a_{j,2}^2} = -\operatorname{sgn}(1) \sqrt{a_{3,2}^2 + a_{4,2}^2} = -\sqrt{1 + \frac{16}{9}} = -\frac{5}{3};$$

$$r = \sqrt{\frac{1}{2}(\alpha^2 - a_{3,2} \cdot \alpha)} = \sqrt{\frac{20}{9}};$$

$$v_1^{(2)} = v_2^{(2)} = 0;$$

$$v_3^{(2)} = \frac{a_{3,2} - \alpha}{2r} = \frac{2}{\sqrt{5}}$$

$$v_4^{(2)} = \frac{a_{4,2}}{2r} = \frac{1}{\sqrt{5}}.$$

and thus new vector  $v$  will be:  $v^{(2)} = (0, 0, \frac{2}{\sqrt{5}}, \frac{1}{\sqrt{5}})^T$  and the new Householder matrix  $P^{(2)}$  will be

$$P^{(2)} = I - 2v^{(2)}(v^{(2)})^T = I - 2 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 4/5 & 2/5 \\ 0 & 0 & 2/5 & 1/5 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -3/5 & -4/5 \\ 0 & 0 & -4/5 & 3/5 \end{bmatrix}$$

and thus

$$A^{(2)} = P^{(2)}A^{(1)}P^{(2)} = \begin{bmatrix} 4 & -3 & 0 & 0 \\ -3 & 10/3 & -5/3 & 0 \\ 0 & -5/3 & -33/25 & 68/75 \\ 0 & 0 & 68/75 & 149/75 \end{bmatrix},$$

As we can see, the final result is a tridiagonal symmetric matrix which is similar to the original one. The process finished after 2 steps.

# Given's Rotation

A Givens rotation is represented by a matrix of the form

$$G(i, j, \theta) = \begin{bmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & c & \cdots & -s & \cdots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & s & \cdots & c & \cdots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix}$$

where  $c = \cos(\theta)$  and  $s = \sin(\theta)$  appear at the intersections  $i$ -th and  $j$ -th rows and columns.

That is, the non-zero elements of Givens matrix is given by:

$$g_{kk} = 1 \quad \text{for } k \neq i, j \quad (3)$$

$$g_{ii} = c \quad (4)$$

$$g_{jj} = c \quad (5)$$

$$g_{ji} = -s \quad (6)$$

$$g_{ij} = s \quad \text{for } i > j \quad (7)$$

(sign of sine switches for  $j > i$ )



## Given's Rotation

The product  $G(i, j, \theta)x$  represents a counterclockwise rotation of the vector  $x$  in the  $(i, j)$  plane of  $\theta$  radians, hence the name Givens rotation. When a Givens rotation matrix  $G$  multiplies another matrix,  $A$ , from the left,  $GA$ , only rows  $i$  and  $j$  of  $A$  are affected. Thus we restrict attention to the following problem. Given  $a$  and  $b$ , find  $c = \cos\theta$  and  $s = \sin\theta$  such that

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}.$$

Explicit calculation of  $\theta$  is rarely necessary or desirable. Instead we directly seek  $c$ ,  $s$ , and  $r$ . An obvious solution would be

$$r = \sqrt{a^2 + b^2} \tag{8}$$

$$c = a/r \tag{9}$$

$$s = -b/r. \tag{10}$$

# Example

Given the following 3x3 Matrix, perform two iterations of the Given's Rotation to bring the matrix to an upper Triangular matrix.

$$A = \begin{bmatrix} 6 & 5 & 0 \\ 5 & 1 & 4 \\ 0 & 4 & 3 \end{bmatrix}$$

In order to form the desired matrix, we must zero elements (2,1) and (3,2). We first select element (2,1) to zero. Using a rotation matrix of:

$$G_1 = \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

We have the following matrix multiplication:

$$A_1 = G_1 \cdot A = \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 6 & 5 & 0 \\ 5 & 1 & 4 \\ 0 & 4 & 3 \end{bmatrix}$$

Where:

$$r = \sqrt{6^2 + 5^2} = 7.8102 \quad (11)$$

$$c = 6/r = 0.7682 \quad (12)$$

$$s = -5/r = -0.6402 \quad (13)$$

Plugging in these values for  $c$  and  $s$  and performing the matrix multiplication above yields a new  $A$  of:

$$A_1 = \begin{bmatrix} 7.8102 & 4.4813 & 2.5607 \\ 0 & -2.4327 & 3.0729 \\ 0 & 4 & 3 \end{bmatrix}$$

We now want to zero element (3,2) to finish off the process. Using the same idea as before, we have a rotation matrix of:

$$G_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & c & -s \\ 0 & s & c \end{bmatrix}$$

We are presented with the following matrix multiplication:

$$A_2 = G_2 \cdot A_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & c & -s \\ 0 & s & c \end{bmatrix} \begin{bmatrix} 7.8102 & 4.4813 & 2.5607 \\ 0 & -2.4327 & 3.0729 \\ 0 & 4 & 3 \end{bmatrix}$$

Where:

$$r = \sqrt{(-2.4327)^2 + 4^2} = 4.6817 \quad (14)$$

$$c = -2.4327/r = -0.5196 \quad (15)$$

$$s = -4/r = -0.8544 \quad (16)$$

Plugging in these values for  $c$  and  $s$  and performing the multiplications gives us a new matrix of:

$$R = A_2 = \begin{bmatrix} 7.8102 & 4.4813 & 2.5607 \\ 0 & 4.6817 & 0.9664 \\ 0 & 0 & -4.1843 \end{bmatrix}$$

# Calculating the QR decomposition

This new matrix  $R$  is the upper triangular matrix needed to perform an iteration of the QR decomposition.  $Q$  is now formed using the transpose of the rotation matrices in the following manner:

$$Q = G_1^T G_2^T$$

We note that

$$G_2 G_1 A = R$$

$$G_1^T G_2^T G_2 G_1 A = G_1^T G_2^T R$$

and thus

$$A = G_1^T G_2^T R = QR$$

with

$$Q = G_1^T G_2^T.$$

Performing this matrix multiplication yields:

$$Q = \begin{bmatrix} 0.7682 & 0.3327 & 0.5470 \\ 0.6402 & -0.3992 & -0.6564 \\ 0 & 0.8544 & -0.5196 \end{bmatrix}$$

## Example

Obtain QR decomposition of the matrix  $A$

$$\mathbf{A} = \begin{bmatrix} 4 & 4 & 3 \\ 3 & 3 & 1 \\ 0 & 4 & 7 \end{bmatrix}$$

using Given's rotation.

Hint:

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}.$$

We directly seek  $c$ ,  $s$ , and  $r$ :

$$r = \sqrt{a^2 + b^2} \quad (17)$$

$$c = a/r \quad (18)$$

$$s = -b/r. \quad (19)$$

To obtain QR decomposition of the matrix  $A$

$$\mathbf{A} = \begin{bmatrix} 4 & 4 & 3 \\ 3 & 3 & 1 \\ 0 & 4 & 7 \end{bmatrix}$$

using Given's rotation we have to zero out (2, 1) and (3, 2) elements of the matrix  $A$ .

1. First, we zero out element (2, 1) of the matrix  $A$ .

To do that we compute  $c, s$  from the known  $a = 4$  and  $b = 3$  as

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

to get formulas:

$$r = \sqrt{a^2 + b^2} = \sqrt{4^2 + 3^2} = 5,$$

$$c = \frac{a}{r} = 0.8,$$

$$s = \frac{-b}{r} = -0.6.$$

The first Given's matrix will be

$$\mathbf{G}_1 = \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

or

$$\mathbf{G}_1 = \begin{bmatrix} 0.8 & 0.6 & 0 \\ -0.6 & 0.8 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Then

$$\mathbf{G}_1 \cdot \mathbf{A} = \begin{bmatrix} 5 & 5 & 3 \\ 0 & 0 & -1 \\ 0 & 4 & 7 \end{bmatrix}$$



2. Next step is to construct second Given's matrix  $G_2$  in order to zero out (3, 2) element of the matrix  $G_1 \cdot A$ .

To do that we compute  $c, s$  from the known  $a = 0$  and  $b = 4$  as

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \cdot \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

to get formulas:

$$r = \sqrt{a^2 + b^2} = \sqrt{0^2 + 4^2} = 4,$$

$$c = \frac{a}{r} = 0,$$

$$s = \frac{-b}{r} = -1.$$

The second Given's matrix will be

$$\mathbf{G}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & c & -s \\ 0 & s & c \end{bmatrix}$$

or

$$\mathbf{G}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$$

Then upper triangular matrix  $R$  in the QR decomposition will be

$$\mathbf{R} = \mathbf{G}_2 \cdot \mathbf{G}_1 \cdot \mathbf{A} = \begin{bmatrix} 5 & 5 & 3 \\ 0 & 4 & 7 \\ 0 & 0 & 1 \end{bmatrix}$$

Then  $A = G_1^T \cdot G_2^T \cdot R = QR$  will be QR decomposition of the matrix  $A$  with  $Q = G_1^T \cdot G_2^T$  given by

$$\mathbf{Q} = \begin{bmatrix} 0.8 & 0 & 0.6 \\ 0.6 & 0 & -0.8 \\ 0 & 1 & 0 \end{bmatrix}$$

# Rank-deficient Least Squares Problems

## Proposition 3.1

Let  $A$  be  $m$  by  $n$  with  $m \geq n$  and  $\text{rank } A = r < n$ . Then there is an  $n - r$  dimensional set of vectors that minimize  $\|Ax - b\|_2$ .

### Proof

Let  $Az = 0$ . Then if  $x$  minimizes  $\|Ax - b\|_2$  then  $x + z$  also minimizes  $\|A(x + z) - b\|_2$ .

This means that the least-squares solution is not unique.

# Moore-Penrose pseudoinverse for a full rank $A$

## Definition

Suppose that  $A$  is  $m$  by  $n$  with  $m > n$  and has full rank with  $A = QR = U\Sigma V^T$  being a  $QR$  and  $SVD$  decompositions of  $A$ , respectively. Then

$$A^+ \equiv (A^T A)^{-1} A^T = R^{-1} Q^T = V \Sigma^{-1} U^T$$

is called the Moore-Penrose pseudoinverse of  $A$ . If  $m < n$  then  $A^+ \equiv A^T (A A^T)^{-1}$ .

The pseudoinverse of  $A$  allows write solution of the full-rank overdetermined least squares problem as  $x = A^+ b$ . If  $A$  is square and a full rank then this formula reduces to  $x = A^{-1} b$ . The  $A^+$  is computed as `pinv(A)` in Matlab.

Moore-Penrose pseudoinverse for rank-deficient  $A$ **Definition**

Suppose that  $A$  is  $m$  by  $n$  with  $m > n$  and is rank-deficient with rank  $r < n$ . Let  $A = U\Sigma V^T = U_1\Sigma_1 V_1^T$  being a SVD decompositions of  $A$  such that

$$A = [U_1, U_2] \left[ \begin{array}{c|c} \Sigma_1 & 0 \\ \hline 0 & 0 \end{array} \right] [V_1, V_2]^T = U_1 \Sigma_1 V_1^T$$

Here,  $\text{size}(\Sigma_1) = r \times r$  and is nonsingular,  $U_1$  and  $V_1$  have  $r$  columns. Then

$$A^+ \equiv V_1 \Sigma_1^{-1} U_1^T$$

is called the Moore-Penrose pseudoinverse for rank-deficient  $A$ . The solution of the least-squares problem is always  $x = A^+ b$ , when  $A$  is rank-deficient then  $x$  has minimum norm.