The QR Algorithm

NORM OF A VECTOR

Norm of a vector $X = \begin{pmatrix} x_1 \\ x_2 \\ . \\ . \\ x_n \end{pmatrix}$ is defined as $\|X\| = \sqrt{x_1^{\ 2} + x_2^{\ 2} + \ldots + x_n^{\ 2}}$

INNER PRODUCT OF TWO COLUMN VECTORS OF SAME ORDER

Inner product of two column vectors A and B of same order is defined as $\langle A, B \rangle = A^T B$

THE MODIFIED GRAM – SCHMIDT PROCESS

Let A be a given matrix having n columns with each of its column vectors denoted by $X_1, X_2, \ldots, X_n$. Then the THE MODIFIED GRAM – SCHMIDT PROCESS is given as follows

The step for kth iteration is given by

STEP 1: Set $r_{kk} = \|X_k\|$ and $Q_k = (1/r_{kk})X_k$

STEP 2: For j = k+1, k+2, ..., n Set $r_{kj} = \langle X_j, Q_k \rangle$

STEP 2: For j = k+1, k+2, ..., n Replace $X_j = X_j - r_{kj}Q_k$

PROBLEMS

1. Construct QR decomposition for the matrix $A = \begin{pmatrix} -4 & 2 & 2 \\ 3 & -3 & 3 \\ 6 & 6 & 0 \end{pmatrix}$

ITERATION 1 (k=1)

$$X_1 = \begin{pmatrix} -4 \\ 3 \\ 6 \end{pmatrix}, X_2 = \begin{pmatrix} 2 \\ -3 \\ 6 \end{pmatrix}, X_3 = \begin{pmatrix} 2 \\ 3 \\ 0 \end{pmatrix}$$

STEP 1: Set $r_{kk} = \|X_k\| \Rightarrow r_{11} = \|X_1\| \Rightarrow r_{11} = \sqrt{(-4)^2 + 3^2 + 6^2} = 7.810250$

and $Q_k = (1/r_{kk})X_k \Rightarrow Q_1 = (1/r_{11})X_1 = (1/7.810250)\begin{pmatrix} -4 \\ 3 \\ 6 \end{pmatrix} = \begin{pmatrix} -0.512148 \\ 0.384111 \\ 0.768221 \end{pmatrix}$

STEP 2: For j = k+1, k+2, ..., n Set $r_{kj} = \langle X_j, Q_k \rangle$

For j = 2,3

$$\Rightarrow r_{12} = \langle X_2, Q_1 \rangle = \begin{pmatrix} 2 \\ -3 \\ 6 \end{pmatrix}^T \begin{pmatrix} -0.512148 \\ 0.384111 \\ 0.768221 \end{pmatrix} = 2.432701.$$

$$\Rightarrow r_{13} = \langle X_3, Q_1 \rangle = \begin{pmatrix} 2 \\ 3 \\ 0 \end{pmatrix}^T \begin{pmatrix} -0.512148 \\ 0.384111 \\ 0.768221 \end{pmatrix} = 0.128037.$$

STEP 3: For j = k+1, k+2, ..., n Replace $X_j = X_j - r_{kj}Q_k$

For j = 2,3

$$X_2 = X_2 - r_{12}Q_1 = \begin{pmatrix} 2 \\ -3 \\ 6 \end{pmatrix} - 2.432701\begin{pmatrix} -0.512148 \\ 0.384111 \\ 0.768221 \end{pmatrix} = \begin{pmatrix} 3.245902 \\ -3.934427 \\ 4.131148 \end{pmatrix}$$

$$X_3 = X_3 - r_{13}Q_1 = \begin{pmatrix} 2 \\ 3 \\ 0 \end{pmatrix} - 0.128037\begin{pmatrix} -0.512148 \\ 0.384111 \\ 0.768221 \end{pmatrix} = \begin{pmatrix} 2.065574 \\ 2.950820 \\ -0.098361 \end{pmatrix}$$

ITERATION 2 (k=2)

STEP 1: Set $r_{kk} = \|X_k\| \Rightarrow r_{22} = \|X_2\|$

$$\Rightarrow r_{22} = \sqrt{(3.245902)^2 + (-3.934427)^2 + 4.131148^2} = 6.563686$$

$$Q_k = (1/r_{kk})X_k \Rightarrow Q_2 = (1/r_{22})X_2 = (1/6.563686)\begin{pmatrix} 3.245902 \\ -3.934427 \\ 4.131148 \end{pmatrix} = \begin{pmatrix} 0.494524 \\ -0.599423 \\ 0.629396 \end{pmatrix}$$

STEP 2: For j = k+1, k+2, ..., n Set $r_{kj} = \langle X_j, Q_k \rangle$

For j = 3

$$\Rightarrow r_{23} = \langle X_3, Q_2 \rangle = \begin{pmatrix} 2.065574 \\ 2.950820 \\ -0.098361 \end{pmatrix}^T \begin{pmatrix} 0.494524 \\ -0.599423 \\ 0.629396 \end{pmatrix} = \text{-0.809221}$$

STEP 3: For j = k+1, k+2, ..., n Replace $X_j = X_j - r_{kj}Q_k$

For j = 3

$$X_3 = X_3 - r_{23}Q_2 = \begin{pmatrix} 2.065574 \\ 2.950820 \\ -0.098361 \end{pmatrix} - (\text{-}0.809221)\begin{pmatrix} 0.494524 \\ -0.599423 \\ 0.629396 \end{pmatrix} = \begin{pmatrix} 2.465753 \\ 2.465754 \\ 0.410960 \end{pmatrix}$$

ITERATION 3 (k=3)

STEP 1: Set $r_{kk} = \|X_k\| \Rightarrow r_{33} = \|X_3\|$

$$\Rightarrow r_{33} = \sqrt{(2.465753)^2 + 2.465754^2 + 0.410960^2} = 3.511235$$

$$Q_k = (1/r_{kk})X_k \Rightarrow Q_3 = (1/r_{33})X_3 = (1/3.511235)\begin{pmatrix} 2.465753 \\ 2.465754 \\ 0.410960 \end{pmatrix} = \begin{pmatrix} 0.702247 \\ 0.702247 \\ 0.117041 \end{pmatrix}$$

$$A = \begin{pmatrix} -0.512148 & 0.494524 & 0.702247 \\ 0.384111 & -0.599423 & 0.702247 \\ 0.768221 & 0.629396 & 0.117041 \end{pmatrix}\begin{pmatrix} 7.810250 & 2.432701 & 0.128037. \\ 0 & 6.563686 & \text{-}0.809221 \\ 0 & 0 & 0 \end{pmatrix}$$

SHIFTED QR DECOMPOSITION

If the matriced have order n x n, then the element in the (n,n) position of A_{k-1} is denoted as s_{k-1} and a QR decomposition is constructed for the shifted matrix

$A_{k-1} - s_{k-1}I = Q_{k-1}R_{k-1}$

and $A_k = R_{k-1}Q_{k-1} + s_{k-1}I$

which constitute the shifted QR algorithm.

Problem

1. Apply shifted QR decomposition for the matrix $A = \begin{pmatrix} 3 & 1 \\ 1 & 5 \end{pmatrix}$

First Iteration

$$\mathbf{A}_0 - 5\mathbf{I} = \begin{bmatrix} -2 & 1 \\ 1 & 0 \end{bmatrix} = \mathbf{Q}_0\mathbf{R}_0 = \begin{bmatrix} -0.894427 & 0.447214 \\ 0.447214 & 0.894427 \end{bmatrix}\begin{bmatrix} 2.236068 & -0.894427 \\ 0 & 0.447124 \end{bmatrix}$$

$$\mathbf{A}_1 = \mathbf{R}_0\mathbf{Q}_0 + 5\mathbf{I} = \begin{bmatrix} 2.236068 & -0.894427 \\ 0 & 0.447214 \end{bmatrix}\begin{bmatrix} -0.894427 & 0.447214 \\ 0.447214 & 0.894427 \end{bmatrix} + 5\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2.6 & 0.2 \\ 0.2 & 5.4 \end{bmatrix}$$

Second Iteration

$$\mathbf{A}_1 - 5.4\mathbf{I} = \begin{bmatrix} -2.8 & 0.2 \\ 0.2 & 0 \end{bmatrix} = \mathbf{Q}_1\mathbf{R}_1 = \begin{bmatrix} -0.997459 & 0.071247 \\ 0.071247 & 0.997459 \end{bmatrix}\begin{bmatrix} 2.807134 & -0.199492 \\ 0 & 0.014249 \end{bmatrix}$$

$$\mathbf{A}_2 = \mathbf{R}_1\mathbf{Q}_1 + 5.4\mathbf{I} = \begin{bmatrix} 2.807134 & -0.199492 \\ 0 & 0.014249 \end{bmatrix}\begin{bmatrix} -0.997459 & 0.071247 \\ 0.071247 & 0.997459 \end{bmatrix} + 5.4\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 2.585787 & 0.001015 \\ 0.001015 & 5.414213 \end{bmatrix}$$

Third iteration

$$\mathbf{A}_2 - 5.414213\mathbf{I} = \begin{bmatrix} -2.828426 & 0.001015 \\ 0.001015 & 0 \end{bmatrix} = \mathbf{Q}_2\mathbf{R}_2 = \begin{bmatrix} -1.000000 & 0.000359 \\ 0.000359 & 1.000000 \end{bmatrix}\begin{bmatrix} 2.828427 & -0.001015 \\ 0 & 0.000000 \end{bmatrix}$$

$$\mathbf{A}_3 = \mathbf{R}_2\mathbf{Q}_2 + 5.414214\mathbf{I} = \begin{bmatrix} 2.828427 & -0.001015 \\ 0 & 0.000000 \end{bmatrix}\begin{bmatrix} -1.000000 & 0.000359 \\ 0.000359 & 1.000000 \end{bmatrix} + 5.414213\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 2.585786 & -0.000000 \\ 0.000000 & 5.414213 \end{bmatrix}$$

Eigen values of A are 2.585786 and 5.144213.

SINGULAR VALUE DECOMPOSITION

Singular Value Decomposition is based on a theorem from linear algebra which says that a rectangular matrix *A* can be broken down into the product of three matrices - an orthogonal matrix *U*, a diagonal matrix *S*, and the transpose of an orthogonal matrix *V*

$$A_{mn} = U_{mm} S_{mn} V_{nn}^T$$

where $U^T U = I$, $V^T V = I$; the columns of *U* are orthonormal eigenvectors of AA^T , the columns of *V* are orthonormal eigenvectors of $A^T A$, and *S* is a diagonal matrix containing the square roots of eigenvalues from *U* or *V* in descending order.

Problem

Construct Singular Value Decomposition of the matrix $A = \begin{pmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{pmatrix}$

In order to find U,

we have to start with AA^T. The transpose of A is

$$A^T = \begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix}$$

$$AA^T = \begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix} \begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 11 & 1 \\ 1 & 11 \end{bmatrix}$$

Next, we have to find the eigenvalues and corresponding eigenvectors of AA^T .

$$\begin{bmatrix} 11 & 1 \\ 1 & 11 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

We rewrite this as the set of equations

$$11x_1 + x_2 = \lambda x_1$$

$$x_1 + 11x_2 = \lambda x_2$$

and rearrange to get

$$(11 - \lambda)x_1 + x_2 = 0$$

$$x_1 + (11 - \lambda)x_2 = 0$$

Solve for λ by setting the determinant of the coefficient matrix to zero,

$$\begin{vmatrix} (11 - \lambda) & 1 \\ 1 & (11 - \lambda) \end{vmatrix} = 0$$

$$(11-\lambda)(11-\lambda)-1\cdot 1=0$$

$$(\lambda-10)(\lambda-12)=0$$

$$\lambda=10, \lambda=12$$

The normalised eigen vectors corresponding to the above eigen values forms U as follows

$$U=\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$

$$A^T A=\begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix}=\begin{bmatrix} 10 & 0 & 2 \\ 0 & 10 & 4 \\ 2 & 4 & 2 \end{bmatrix}$$

Proceeding in similar manner

$$A^T A=\begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix}=\begin{bmatrix} 10 & 0 & 2 \\ 0 & 10 & 4 \\ 2 & 4 & 2 \end{bmatrix}$$

The normalised eigen vectors corresponding to the eigen values of the above matrix forms V as follows

$$V=\begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{30}} \\ \frac{2}{\sqrt{6}} & \frac{-1}{\sqrt{5}} & \frac{2}{\sqrt{30}} \\ \frac{1}{\sqrt{6}} & 0 & \frac{-5}{\sqrt{30}} \end{bmatrix}$$

$$V^T=\begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{bmatrix}$$

For S we take the square roots of the non-zero eigenvalues and populate the diagonal with them, putting the largest in s_{11}, the next largest in s_{22} and so on until the smallest value ends up in s_{mm}. The non-zero eigenvalues of U and V are always the same, so that's why it doesn't matter which one we take them from.

$$S=\begin{bmatrix} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{bmatrix}$$

$$A_{mn}=U_{mm}S_{mn}V_{nn}^T=\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}\begin{bmatrix} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{bmatrix}\begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{bmatrix}$$

PSEUDO INVERSE OR GENERALISED INVERSE OF A MATRIX

Procedure:

Let A be a given matrix of order m x n. Let the rank of matrix of A be 'k'. Find a submatrix of A of rank 'k' and order k x k. Through a sequence of elementary row and column operations of the first kind move the submatrix identitied in previous step in to the upper left portion of A. That is determine

$$PAQ = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

where P and Q are each the product of elementary matrices of the first kind, and $A_{11}$is a submatrix of A that is non-singular and of rank k. If no elementary operations were necessary then P and Q are identity matrices. A_{12}, A_{21}, A_{22} may be empty.

Set $B = \begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}$, $F = A_{11}^{-1} A_{12}$, $C = [I_K / F]$, where I_k is the k x k identity matrix.

$$A^{+} = QC^H (CC^H)^{-1} (B^H B)^{-1} B^H P$$

If all the columns of A are independent then

$$A^{+} = (A^H A)^{-1} A^H$$

Problems

Find Generalised inverse of the matrix

$$\mathbf{A} = \begin{bmatrix} 2 & 2 & -2 \\ 2 & 2 & -2 \\ -2 & -2 & 6 \end{bmatrix}$$

$$\mathbf{P} = \mathbf{Q} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad \text{gives us} \quad \mathbf{PAQ} = \left[\begin{array}{cc:c} 2 & -2 & 2 \\ -2 & 6 & -2 \\ \hdashline 2 & -2 & 2 \end{array}\right]$$

where $\mathbf{A}_{11} = \begin{bmatrix} 2 & -2 \\ -2 & 6 \end{bmatrix}$ $\mathbf{A}_{12} = \begin{bmatrix} 2 \\ -2 \end{bmatrix}$ and $\mathbf{A}_{21} = [2, -2]$

and $\mathbf{A}_{11}$ has rank 2. Then

$$\mathbf{B} = \left[\begin{array}{cc} 2 & -2 \\ -2 & 6 \\ \hdashline 2 & -2 \end{array}\right] \quad \mathbf{F} = \mathbf{A}_{11}^{-1}\mathbf{A}_{12} = \begin{bmatrix} 6/8 & 2/8 \\ 2/8 & 2/8 \end{bmatrix}\begin{bmatrix} 2 \\ -2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \mathbf{C} = \left[\begin{array}{cc:c} 1 & 0 & 1 \\ 0 & 1 & 0 \end{array}\right]$$

so $(\mathbf{CC}^H)^{-1} = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1/2 & 0 \\ 0 & 1 \end{bmatrix}$ and $(\mathbf{B}^H\mathbf{B})^{-1} = \begin{bmatrix} 12 & -20 \\ -20 & 44 \end{bmatrix}^{-1} = \begin{bmatrix} 11/32 & 5/32 \\ 5/32 & 3/32 \end{bmatrix}$

and

$$\mathbf{A}^{+} = \mathbf{QC}^H(\mathbf{CC}^H)^{-1}(\mathbf{B}^H\mathbf{B})^{-1}\mathbf{B}^H\mathbf{P}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1/2 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 11/32 & 5/32 \\ 5/32 & 3/32 \end{bmatrix}\begin{bmatrix} 2 & -2 & 2 \\ -2 & 6 & -2 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 3/16 & 3/16 & 1/8 \\ 3/16 & 3/16 & 1/8 \\ 1/8 & 1/8 & 1/4 \end{bmatrix}$$

SOLUTION TO LINEAR EQUATIONS BY LEAST SQUARE APPROXIMATIONS

A least square solution to a set of simultaneous linear equations AX = B is the vector of smallest Euclidean norm that minimizes $\|AX - B\|_2$. That vector is $X = A^+B$.

Problem

Solve the following system of equations in the least square sense

$2x_1 + 2x_2 - 2x_3 = 1$, $2x_1 + 2x_2 - 2x_3 = 3$, $-2x_1 - 2x_2 + 6x_3 = 2$.

The above system of equation is an inconsistent one. Rewriting the equation in matrix form and taking generalised inverse of the coefficient matrix we get the following least square approximation.

$$\Rightarrow \begin{pmatrix} 2 & 2 & -2 \\ 2 & 2 & -2 \\ -2 & -2 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 2 & 2 & -2 \\ 2 & 2 & -2 \\ -2 & -2 & 6 \end{pmatrix}^+ \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 2 & 2 & -2 \\ 2 & 2 & -2 \\ -2 & -2 & 6 \end{pmatrix}^+ \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3/16 & 3/16 & 1/8 \\ 3/16 & 3/16 & 1/8 \\ 1/8 & 1/8 & 1/4 \end{pmatrix}^+ \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Note: The generalised inverse of the matrix is already found in previous section which is used in the above step.

Hence the Least Square solution is given by

$x_1 = 1$

$x_2 = 1$

$x_3 = 1$