NA15 QR rastav

Ivan Slapničar

3. prosinca 2018.

1 QR rastav

QR rastav matrice *A* tipa $m \times n$, $m \ge n$, glasi

$$A = QR$$
,

pri čemu je Q ortonormirana matrica dimenzije $m \times m$, odnosno

$$Q^T Q = Q Q^T = I,$$

a R je $m \times n$ gornje trokutasta matrica.

Ortonormiranu matricu kraće zovemo i ortogonalna matrica.

Na primjer,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \\ a_{51} & a_{52} & a_{53} \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} & q_{13} & q_{14} & q_{15} \\ q_{21} & q_{22} & q_{23} & q_{24} & q_{25} \\ q_{31} & q_{32} & q_{33} & q_{34} & q_{35} \\ q_{41} & q_{42} & q_{43} & q_{44} & q_{45} \\ q_{51} & q_{52} & q_{53} & q_{54} & q_{55} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$
 (1)

S (1) je definiram i ekonomični QR rastav

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \\ a_{51} & a_{52} & a_{53} \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \\ q_{41} & q_{42} & q_{43} \\ q_{51} & q_{52} & q_{53} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \end{bmatrix}.$$

$$(2)$$

Izjednačavanje stupaca počevši od prvog daje:

$$t = a_{:1}$$

$$r_{11} = ||t||_{2}$$

$$q_{:1} = t \frac{1}{r_{11}}$$

$$r_{12} = q_{:1}^{T} a_{:1}$$

$$t = a_{:2} - q_{:1} r_{12}$$

$$r_{22} = ||t||_{2}$$

$$q_{:2} = t \frac{1}{r_{22}}$$

$$r_{13} = q_{:1}^{T} a_{:3}$$

$$r_{23} = q_{:2}^{T} a_{:3}$$

$$t = a_{:3} - q_{:1} r_{13} - q_{:2} r_{23}$$

$$r_{33} = ||t||_{2}$$

$$q_{:3} = t \frac{1}{r_{33}}$$

Indukcijom slijedi Gram-Schmidtov postupak ortogonalizacije.

```
In [1]: using LinearAlgebra
        function myGramSchmidtQR(A::Array)
            m,n=size(A)
            R=zeros(n,n)
            Q=Array{Float64}(undef,m,n)
            R[1,1]=norm(A[:,1])
            Q[:,1]=A[:,1]/R[1,1]
            for k=2:n
                for i=1:k-1
                    R[i,k]=Q[:,i]\cdot A[:,k]
                end
                t=A[:,k]-sum([R[i,k]*Q[:,i] for i=1:k-1])
                R[k,k]=norm(t)
                Q[:,k]=t/R[k,k]
            end
            Q,R
        end
Out[1]: myGramSchmidtQR (generic function with 1 method)
In [2]: import Random
        Random.seed! (123)
        A=rand(8,5)
Out[2]: 8×5 Array{Float64,2}:
         0.768448
                    0.26864 0.275819 0.20923 0.356221
```

```
0.108871 0.446568 0.918165 0.900925
        0.673959
                   0.163666 0.582318 0.614255 0.529253
        0.395453
                   0.473017 0.255981 0.802665 0.031831
                   0.865412 0.70586
                                      0.555668 0.900681
        0.313244
        0.662555
                   0.617492 0.291978 0.940782 0.940299
        0.586022
                   0.285698 0.281066 0.48
                                                0.621379
        0.0521332  0.463847  0.792931  0.790201  0.348173
In [3]: Q,R=myGramSchmidtQR(A)
Out[3]: ([0.445979 -0.112473 ... -0.581217 -0.414126; 0.545841 -0.354798 ...
0.296518 \ 0.303573; \dots; 0.340106 \ -0.00596216 \dots \ -0.076101 \ 0.141458;
0.0302562 0.432357 ... 0.25137 -0.128359], [1.72306 0.857781 ...
1.66889 1.61212; 0.0 1.01281 ... 0.760568 0.603988; ...; 0.0 0.0 ...
0.686493 -0.00271451; 0.0 0.0 ... 0.0 0.652889])
In [4]: Q
Out[4]: 8×5 Array{Float64,2}:
        0.445979
                   -0.112473
                                -0.144567
                                           -0.581217
                                                       -0.414126
                                                        0.303573
        0.545841
                   -0.354798
                                 0.210356
                                            0.296518
        0.391141
                  -0.169675
                                 0.45213
                                            -0.0982655 -0.123261
        0.229507
                 0.272659
                             -0.24854
                                            0.435716
                                                       -0.699857
        0.181796
                  0.700501
                                 0.0463297 -0.432191
                                                       0.268038
        0.384523 0.284018
                                -0.440047
                                            0.344953
                                                        0.350741
        0.340106 -0.00596216 -0.0882082 -0.076101
                                                        0.141458
        0.0302562 0.432357
                                 0.681975
                                            0.25137
                                                       -0.128359
In [5]: Q'*Q
Out [5]: 5\times5 Array{Float64,2}:
         1.0
                       7.28584e-17 -3.81639e-17 4.96131e-16
                                                                2.77556e-16
         7.28584e-17 1.0
                                    -5.55112e-17 -2.35922e-16 -5.55112e-17
        -3.81639e-17 -5.55112e-17
                                   1.0
                                                  1.11022e-16
                                                                2.39392e-16
         4.96131e-16 -2.35922e-16 1.11022e-16
                                                               -1.02696e-15
                                                 1.0
         2.77556e-16 -5.55112e-17 2.39392e-16 -1.02696e-15
                                                                1.0
In [6]: R
Out[6]: 5×5 Array{Float64,2}:
        1.72306 0.857781 1.01346
                                     1.66889
                                               1.61212
        0.0
                 1.01281
                           0.700064 0.760568
                                               0.603988
        0.0
                 0.0
                           0.67391
                                     0.349435
                                               0.179984
                 0.0
                           0.0
                                     0.686493 -0.00271451
        0.0
        0.0
                 0.0
                           0.0
                                     0.0
                                               0.652889
In [7]: # Rezidual
```

0.940515

A-Q*R

Out[7]: 8×5 Array{Float64,2}:

Algoritam myGramSchmidtQR() je numerički nestabilan pa je bolje koristiti modificirani Gram-Schmidtov algoritam ili Householderove reflektore ili Givensove rotacije (vidi Matrix Computations, poglavlje 5).

1.1 Householderovi reflektori

QR rastav vektora x jednak je

$$H\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} = r,$$

gdje je

$$H = I - rac{2}{v^T v} v v^T, \qquad v = egin{bmatrix} x_1 \pm \|x\|_2 \ x_2 \ x_3 \ dots \ x_m \end{bmatrix}.$$

Householderov reflektor H je *simetrična* i *ortogonalna* matrica (dokažite!). Ovisno o izboru predznaka u definicije vektora *v* vrijedi

$$r = \begin{bmatrix} \mp \|x\| \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Zbog numeričke stabilnost se najčešće uzima

$$v_1 = x_1 + \text{sign}(x_1) ||x||_2.$$

Matrica H se ne računa eksplicitno već se produkt Hx računa po formuli

$$Hx = x - \frac{2(v^T x)}{v^T v} v = x - \frac{2(v \cdot x)}{v \cdot v} v$$

za koju je potrebno O(6m) operacija.

```
In [8]: function myHouseholderVector(x::Array)
             # Racuna v
             v=deepcopy(x)
             v[1]=x[1]+sign(x[1])*norm(x)
         end
Out[8]: myHouseholderVector (generic function with 1 method)
In [9]: x=rand(8)
        v=myHouseholderVector(x)
        \beta = (2/(v \cdot v)) * (v \cdot x)
        x-\beta*v
Out[9]: 8-element Array{Float64,1}:
          -1.2568320365216425
           0.0
           0.0
           0.0
           0.0
           0.0
           0.0
           0.0
In [10]: norm(x)
Out[10]: 1.2568320365216425
```

QR rastav matrice se računa rekurzivnim QR rastavom vektora pomoću Householderovih reflektora:

```
Out[11]: myHouseholderQR (generic function with 1 method)
In [12]: A
Out[12]: 8×5 Array{Float64,2}:
         0.768448
                  0.26864
                            0.275819 0.20923
                                              0.356221
         0.940515
                  0.108871 0.446568 0.918165
                                              0.900925
         0.031831
         0.313244
                  0.865412 0.70586
                                     0.555668
                                              0.900681
         0.662555
                  0.617492 0.291978 0.940782
                                              0.940299
         0.586022
                  0.285698 0.281066 0.48
                                              0.621379
         0.0521332  0.463847  0.792931  0.790201  0.348173
In [13]: Q,R=myHouseholderQR(A)
Out[13]: ([-0.445979 -0.112473 ... -0.184609 0.445399; -0.545841 -0.354798 ...
-0.284531 \ 0.161726; \dots; -0.340106 \ -0.00596216 \dots 0.911612 \ 0.0807266;
-0.0302562 0.432357 ... 0.0808767 0.47278], [-1.72306 -0.857781 ...
-1.66889 -1.61212; 0.0 1.01281 ... 0.760568 0.603988; ... ;
In [14]: Q'*A
Out[14]: 8×5 Array{Float64,2}:
         -1.72306
                     -0.857781
                                  -1.01346
                                               -1.66889
                                                           -1.61212
         1.45717e-16
                     1.01281
                                   0.700064
                                               0.760568
                                                            0.603988
          2.08167e-17 -5.55112e-17 -0.67391
                                               -0.349435
                                                           -0.179984
         -6.07153e-17 -2.77556e-17 8.32667e-17 -0.686493
                                                            0.00271451
          1.83881e-16 2.70617e-16
                                   2.91434e-16 1.38778e-16 -0.652889
         2.94903e-17
                      5.55112e-17
                                   1.11022e-16
                                               1.11022e-16
                                                            1.11022e-16
         -2.42861e-17
                      6.93889e-18 5.55112e-17
                                               4.16334e-17 -1.11022e-16
          3.1225e-17
                      0.0
                                   5.55112e-17
                                                            0.0
                                               0.0
In [15]: R
Out[15]: 8×5 Array{Float64,2}:
         -1.72306 -0.857781 -1.01346
                                      -1.66889
                                                -1.61212
          0.0
                   1.01281
                             0.700064
                                       0.760568
                                                0.603988
          0.0
                  0.0
                            -0.67391
                                      -0.349435
                                               -0.179984
          0.0
                  0.0
                            0.0
                                      -0.686493
                                                0.00271451
                                      0.0
          0.0
                  0.0
                            0.0
                                                -0.652889
          0.0
                  0.0
                            0.0
                                       0.0
                                                0.0
          0.0
                  0.0
                            0.0
                                       0.0
                                                0.0
         0.0
                                       0.0
                                                0.0
                  0.0
                            0.0
```

Program myHouseholderQR() je ilustrativan. Profesionalni programi imaju sljedeća svojstva:

- računaju s blok matricama (uobičajena dimenzija bloka je 32 ili 64),
- izračuna se vektor $\hat{v} = v/v_1$. Vrijedi $\hat{v}_1 = 1$, dok se ostali elemenenti vektora \hat{v} spremaju u strogi donji trokut matrice A,
- ako se traži matrica Q, akumulacija se vrši unatrag koristeći spremljene vektore v (tako se smanjuje broj operacija),
- postoji opcija vraćanja ekonomičnog rastava,
- postoji opcija računanja s *pivotiranjem* u svakom koraku se na prvo mjesto dovede stupac s najvećom normom pa je

$$AP = QR$$
.

Vrijedi

$$|R_{kk}| \geq |R_{k+1,k+1}|$$

pa se može utvrditi i numerički rank matrice.

```
In [16]: # ?qr
In [17]: F=qr(A)
Out[17]: LinearAlgebra.QRCompactWY{Float64,Array{Float64,2}}
         Q factor:
         8×8 LinearAlgebra.QRCompactWYQ{Float64,Array{Float64,2}}:
          -0.445979
                      -0.112473
                                     0.144567
                                                      0.160558 -0.184609
                                                                              0.445399
                      -0.354798
          -0.545841
                                    -0.210356
                                                   -0.494706 -0.284531
                                                                            0.161726
          -0.391141
                      -0.169675
                                    -0.45213
                                                    0.385539
                                                               0.0148903 -0.66339
          -0.229507
                       0.272659
                                    0.24854
                                                   -0.295448
                                                               0.0184688 -0.209603
                                                   -0.362887 -0.160778
          -0.181796
                       0.700501
                                    -0.0463297
                                                                           -0.240692
          -0.384523
                       0.284018
                                    0.440047
                                                      0.558011 -0.144818
                                                                              0.0589447
          -0.340106
                      -0.00596216
                                     0.0882082
                                                   -0.114703
                                                               0.911612
                                                                            0.0807266
          -0.0302562
                       0.432357
                                    -0.681975
                                                    0.193228
                                                               0.0808767
                                                                            0.47278
         R factor:
         5 \times 5 Array{Float64,2}:
          -1.72306 -0.857781 -1.01346
                                           -1.66889
                                                      -1.61212
           0.0
                     1.01281
                                0.700064
                                            0.760568
                                                       0.603988
           0.0
                     0.0
                               -0.67391
                                           -0.349435 -0.179984
           0.0
                     0.0
                                0.0
                                           -0.686493
                                                       0.00271451
           0.0
                     0.0
                                0.0
                                            0.0
                                                      -0.652889
```

In [18]: F.Q'*A

Out[18]: 8×5 Array{Float64,2}:

```
-1.72306 -0.857781 -1.01346 -1.66889 -1.61212
-1.11022e-16 1.01281 0.700064 0.760568 0.603988
-1.11022e-16 2.77556e-17 -0.67391 -0.349435 -0.179984
```

```
-2.77556e-16 -1.66533e-16 -3.33067e-16 -0.686493
                                                                0.00271451
         -3.88578e-16
                      1.11022e-16
                                                 -2.22045e-16 -0.652889
                                   0.0
         -3.33067e-16 -1.11022e-16 -1.11022e-16 -2.22045e-16
                                                               1.11022e-16
          0.0
                       0.0
                                     0.0
                                                  0.0
                                                                1.11022e-16
                       5.55112e-17 -1.11022e-16 -1.11022e-16 -5.55112e-17
         -1.94289e-16
In [19]: F.Q*F.R
Out[19]: 8×5 Array{Float64,2}:
         0.768448
                    0.26864
                             0.275819 0.20923
                                                 0.356221
         0.940515
                    0.108871 0.446568 0.918165
                                                0.900925
         0.673959
                                                0.529253
                    0.163666 0.582318 0.614255
         0.395453
                    0.473017 0.255981 0.802665
                                                0.031831
         0.313244
                    0.865412 0.70586
                                       0.555668
                                                0.900681
         0.662555
                    0.617492 0.291978 0.940782
                                                0.940299
         0.586022
                    0.285698 0.281066 0.48
                                                 0.621379
         In [20]: F=qr(A, Val(true))
Out[20]: QRPivoted{Float64,Array{Float64,2}}
        Q factor:
        8×8 LinearAlgebra.QRPackedQ{Float64,Array{Float64,2}}:
                                           . . .
                                               -0.418105
         -0.105181 -0.657376
                               -0.16259
                                                           -0.280647
                                                                       -0.0682982
         -0.461568 -0.291448
                                0.0230722
                                              -0.0183557 -0.262798
                                                                      0.531458
         -0.30879
                   -0.242706
                               -0.109412
                                               0.57546
                                                          0.1056
                                                                     -0.496631
         -0.403505
                    0.200334
                               -0.681506
                                               0.246128
                                                          0.0857566
                                                                      0.252251
         -0.279338
                     0.0965824
                                0.643895
                                               0.323668
                                                         -0.0771281
                                                                      0.323665
         -0.472938
                     0.0225186
                                                -0.117048
                                0.243739
                                                           -0.204861
                                                                       -0.529297
         -0.241299 -0.252973
                                0.145506
                                              -0.246011
                                                          0.885934
                                                                      0.0728644
         -0.397239
                     0.556817
                               -0.0378098
                                              -0.504117
                                                         -0.0295477 -0.111318
        R factor:
        5\times5 Array{Float64,2}:
         -1.98923 -1.44558
                                        -1.10689
                                                   -1.2363
                             -1.61412
          0.0
                   -0.937667 -0.473979
                                         0.130204
                                                   0.0436452
                              0.76965
          0.0
                    0.0
                                         0.350337
                                                   0.263875
          0.0
                    0.0
                              0.0
                                        -0.629825
                                                  -0.177484
          0.0
                    0.0
                              0.0
                                         0.0
                                                   -0.582983
        permutation:
        5-element Array{Int64,1}:
         1
         5
         2
         3
In [21]: # Vektor pivotiranja
```

F.p

```
Out[21]: 5-element Array{Int64,1}:
         4
         1
         5
         2
         3
In [22]: # Matrica pivotiranja
        F.P
Out[22]: 5×5 Array{Float64,2}:
         0.0 1.0 0.0 0.0 0.0
         0.0 0.0 0.0 1.0 0.0
         0.0 0.0 0.0 0.0 1.0
         1.0 0.0 0.0 0.0 0.0
         0.0 0.0 1.0 0.0 0.0
In [23]: # Provjera s matricom
        F.Q*F.R-A*F.P
Out[23]: 8×5 Array{Float64,2}:
         0.0
                     8.88178e-16 4.44089e-16
                                               2.22045e-16 4.44089e-16
         0.0
                     4.44089e-16 3.33067e-16 -1.11022e-16 1.11022e-16
         0.0
                     3.33067e-16 1.11022e-16 8.32667e-17 0.0
         0.0
                     2.77556e-16 1.11022e-16 2.22045e-16 5.55112e-17
         0.0
                     3.33067e-16 0.0
                                               2.22045e-16 2.22045e-16
         1.11022e-16 4.44089e-16 2.22045e-16 2.22045e-16 3.33067e-16
         5.55112e-17 2.22045e-16 1.11022e-16
                                               0.0
                                                            1.11022e-16
         1.11022e-16 1.11022e-16 5.55112e-17
                                               2.77556e-16 2.22045e-16
In [24]: # Provjera s vektorom
        F.Q*F.R-A[:,F.p]
Out[24]: 8×5 Array{Float64,2}:
         0.0
                     8.88178e-16 4.44089e-16 2.22045e-16 4.44089e-16
         0.0
                     4.44089e-16 3.33067e-16 -1.11022e-16 1.11022e-16
         0.0
                     3.33067e-16 1.11022e-16 8.32667e-17 0.0
                     2.77556e-16 1.11022e-16 2.22045e-16 5.55112e-17
         0.0
         0.0
                     3.33067e-16 0.0
                                               2.22045e-16 2.22045e-16
         1.11022e-16 4.44089e-16 2.22045e-16 2.22045e-16 3.33067e-16
         5.55112e-17 2.22045e-16 1.11022e-16
                                               0.0
                                                            1.11022e-16
         1.11022e-16 1.11022e-16 5.55112e-17
                                               2.77556e-16 2.22045e-16
```

1.2 Brzina

Broj računskih operacija potrebnih za računanje QR rastava matrice $n \times n$ je $O(\frac{4}{3}n^3)$ za računanje matrice Q.

1.3 Točnost

Za matrice \hat{Q} i \hat{R} izračunate Householder-ovom metodom vrijedi:

$$\hat{Q}^T \hat{Q} = I + E, \qquad ||E||_2 \approx \varepsilon,$$

$$||A - \hat{Q}\hat{R}||_2 \approx \varepsilon ||A||_2.$$

Također, postoji egzaktna ortogonalna matrica Q za koju je

$$||A - Q\hat{R}||_2 \approx \varepsilon ||A||_2.$$