### PracticeSession07

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# Numerical Linear Algebra for Computational Science and Information Engineering

#### Orthogonalization and Least-Squares Problems

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 $A = U[:, 1:n] * \Sigma * V'$ 

return A

end:

```
Fandom, SparseArrays

[2]: function conditioned_matrix(m::Int, n::Int, cond::Float64)

U, _ = qr(randn(m, m))

V, _ = qr(randn(n, n))

s = range(1.0, 1/cond; length=n)

Σ = Diagonal(s)
```

[1]: using LinearAlgebra, Plots, Printf, Latexify, LaTeXStrings, BenchmarkTools,

### Exercise #1: Implement and test your implementation of HouseholderQR

```
[3]: function HouseholderQR(A)
    m, n = size(A)
    Q = Matrix{Float64}(I, m, m)
    R = copy(A)
    for k = 1:n
        # Compute Householder vector
        v = R[k:m, k]
        v[1] -= sign(v[1]) * norm(v) # usage of sign(v[1]) allows to prevent
        catastrophic cancellation
        beta = 2. / v'v
        # Apply Householder reflection
        R[k:m, k:n] -= beta .* v * (v'R[k:m, k:n])
        Q[1:m, k:m] -= Q[1:m, k:m] * v * (beta .* v')
        end
        return Q, R
end;
```

```
[4]: m = 1_000;
     n = 200;
     Random.seed!(3);
     A1 = conditioned_matrix(m, n, 1e8);
     A2 = conditioned_matrix(m, n, 1e10);
[5]: Q, R = Obtime HouseholderQR(A1);
     2.437 s (7807 allocations: 5.94 GiB)
    ||A - QR|| = 1.15E-14, ||I - Q'Q|| = 4.62E-14
[6]: Q, R = Obtime HouseholderQR(A2);
     2.519 s (7807 allocations: 5.94 GiB)
    ||A - QR|| = 1.09E-14, ||I - Q'Q|| = 4.54E-14
    Exercise #2: Implement CholeskyQR, CholeskyQR2 and Shifted CholeskyQR3
[7]: function CholeskyQR(A)
      X = A \cdot A
      chol = cholesky(X)
      Q = A / chol.U
      return Q, chol.U
     end;
[8]: function CholeskyQR2(A)
      Q1, R1 = CholeskyQR(A)
      Q, R2 = CholeskyQR(Q1)
      return Q, R2 * R1
     end;
[9]: function ShiftedCholeskyQR(A)
      X = A'A
      s = 11 * (m * n + n * (n + 1)) * eps() * norm(A)
      X += s * I
      chol = cholesky(X)
      Q = A / chol.U
      return Q, chol.U
     end;
[10]: function ShiftedCholeskyQR3(A)
      Q1, R1 = ShiftedCholeskyQR(A)
      Q, R2 = CholeskyQR2(Q1)
      return Q, R2 * R1
     end;
```

# Exercise #3: Compare loss of orthogonality and residual of each CholeskyQR implementation

```
[11]: Q, R = Obtime CholeskyQR(A1);
          Q_{P} Q_{P
            2.357 ms (10 allocations: 2.14 MiB)
         ||A - QR|| = 9.30E-16, ||I - Q'Q|| = 2.77E-02
[12]: Q, R = Obtime CholeskyQR(A2);
          PosDefException: matrix is not positive definite; Factorization failed.
           Stacktrace:
              [1] checkpositivedefinite
                  @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
             [2] #cholesky!#163
                  @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
             →LinearAlgebra/src/cholesky.jl:269 [inlined]
              [3] cholesky!
                 @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/

→LinearAlgebra/src/cholesky.jl:267 [inlined]

              [4] #cholesky!#164
                 @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/

→LinearAlgebra/src/cholesky.jl:301 [inlined]

              [5] cholesky! (repeats 2 times)
                  @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
             →LinearAlgebra/src/cholesky.jl:295 [inlined]
              [6] cholesky
                  @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
             →LinearAlgebra/src/cholesky.jl:411 [inlined]
              [7] cholesky(A::Matrix{Float64}, ::NoPivot; check::Bool)
                  @ LinearAlgebra ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/
             ⇒stdlib/v1.11/LinearAlgebra/src/cholesky.jl:401
              [8] cholesky (repeats 2 times)
                  @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
             [9] CholeskyQR(A::Matrix{Float64})
                  @ Main ./In[7]:3
             [10] var"##core#256"()
                  @ Main ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:598
             [11] var"##sample#257"(::Tuple{}, __params::BenchmarkTools.Parameters)
                  @ Main ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:607
             [12] lineartrial(b::BenchmarkTools.Benchmark, p::BenchmarkTools.Parameters;
             →maxevals::Int64, kwargs::@Kwargs{})
                  @ BenchmarkTools ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:18
```

```
[13] lineartrial(b::BenchmarkTools.Benchmark, p::BenchmarkTools.Parameters)
                            @ BenchmarkTools ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:18
                    [14] #invokelatest#2
                            @ ./essentials.jl:1055 [inlined]
                    [15] invokelatest
                            @ ./essentials.jl:1052 [inlined]
                    [16] #lineartrial#46
                            @ ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:51 [inlined]
                    [17] lineartrial
                            @ ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:50 [inlined]
                    [18] tune!(b::BenchmarkTools.Benchmark, p::BenchmarkTools.Parameters;
                     progressid::Nothing, nleaves::Float64, ndone::Float64, verbose::Bool, pad::
                     ⇔String, kwargs::@Kwargs{})
                            @ BenchmarkTools ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:29
                    [19] tune!
                            @ ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:288 [inlined]
                    [20] tune!(b::BenchmarkTools.Benchmark)
                            @ BenchmarkTools ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:28
                    [21] top-level scope
                            @ ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:728
[13]: Q, R = Obtime CholeskyQR2(A1);
               Q_{P} Q_{P
                   4.780 ms (22 allocations: 4.58 MiB)
              ||A - QR|| = 3.35E-15, ||I - Q'Q|| = 5.57E-15
[14]: Q, R = Obtime CholeskyQR2(A2);
               Q_{P_{A}} Q_{P
                 PosDefException: matrix is not positive definite; Factorization failed.
                 Stacktrace:
                       [1] checkpositivedefinite
                            @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
                     →LinearAlgebra/src/factorization.jl:68 [inlined]
                       [2] #cholesky!#163
                            @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
                     □ LinearAlgebra/src/cholesky.jl:269 [inlined]
                       [3] cholesky!
                            @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
                     [4] #cholesky!#164
                            @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
                     →LinearAlgebra/src/cholesky.jl:301 [inlined]
                       [5] cholesky! (repeats 2 times)
```

```
@ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
→LinearAlgebra/src/cholesky.jl:295 [inlined]
[6] _cholesky
  @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
→LinearAlgebra/src/cholesky.jl:411 [inlined]
[7] cholesky(A::Matrix{Float64}, ::NoPivot; check::Bool)
  @ LinearAlgebra ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/
⇒stdlib/v1.11/LinearAlgebra/src/cholesky.jl:401
 [8] cholesky (repeats 2 times)
  @ ~/.julia/juliaup/julia-1.11.5+0.x64.linux.gnu/share/julia/stdlib/v1.11/
→LinearAlgebra/src/cholesky.jl:401 [inlined]
[9] CholeskyQR(A::Matrix{Float64})
  @ Main ./In[7]:3
[10] CholeskyQR2(A::Matrix{Float64})
   @ Main ./In[8]:2
[11] var"##core#270"()
  @ Main ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:598
[12] var"##sample#271"(::Tuple{}, __params::BenchmarkTools.Parameters)
  @ Main ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:607
[13] lineartrial(b::BenchmarkTools.Benchmark, p::BenchmarkTools.Parameters;
→maxevals::Int64, kwargs::@Kwargs{})
  @ BenchmarkTools ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:18
[14] _lineartrial(b::BenchmarkTools.Benchmark, p::BenchmarkTools.Parameters)
  @ BenchmarkTools ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:18
[15] #invokelatest#2
  @ ./essentials.jl:1055 [inlined]
[16] invokelatest
  @ ./essentials.jl:1052 [inlined]
[17] #lineartrial#46
  @ ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:51 [inlined]
[18] lineartrial
   @ ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:50 [inlined]
[19] tune!(b::BenchmarkTools.Benchmark, p::BenchmarkTools.Parameters;
progressid::Nothing, nleaves::Float64, ndone::Float64, verbose::Bool, pad::

→String, kwargs::@Kwargs{})
  @ BenchmarkTools ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:29
[20] tune!
  @ ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:288 [inlined]
[21] tune!(b::BenchmarkTools.Benchmark)
   @ BenchmarkTools ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:28
[22] top-level scope
  @ ~/.julia/packages/BenchmarkTools/1i1mY/src/execution.jl:728
```

7.750 ms (51 allocations: 7.33 MiB)

#### Exercise #4: Implement CGS, MGS and CGS2

```
[17]: function CGS_naive(X::Array{Float64,2})
       n, m = size(X)
        Q = Array{Float64,2}(undef, n, m)
        R = zeros(Float64, m, m)
        R[1, 1] = norm(X[:, 1])
        Q[:, 1] = X[:, 1] ./ R[1, 1]
        for i in 2:m
          Q[:, i] = X[:, i]
          R[1:i-1, i] = Q[:, 1:i-1]'X[:, i] # creates temporary array => very slow
          Q[:, i] = Q[:, 1:i-1] * R[1:i-1, i] # creates temporary array => very slow
          R[i, i] = norm(Q[:, i])
          Q[:, i] ./= R[i, i]
        end
        return Q, R
      end;
      function CGS(X::Array{Float64,2})
        n, m = size(X)
        Q = zeros(Float64, n, m)
        R = zeros(Float64, m, m)
        r = zeros(Float64, m)
        w = zeros(Float64, n)
        R[1, 1] = norm(X[:, 1])
        Q[:, 1] = X[:, 1] ./ R[1, 1]
        for i in 2:m
          w := X[:, i]
          r .= (w'Q)'
          r[i:m] = 0.
          R[:, i] = r
          w -= Q * r
          R[i, i] = norm(w)
          Q[:, i] = w ./ R[i, i]
        end
        return Q, R
      end;
```

```
[18]: function MGS_naive(X::Array{Float64,2})
    n, m = size(X)
```

```
Q = Array{Float64,2}(undef, n, m)
  R = zeros(Float64, m, m)
  R[1, 1] = norm(X[:, 1])
  Q[:, 1] = X[:, 1] ./ R[1, 1]
  for i in 2:m
    Q[:, i] = X[:, i]
    for j in 1:i-1
      R[j, i] = Q[:, j]'Q[:, i]
      Q[:, i] = R[j, i] .* Q[:, j]
    R[i, i] = norm(Q[:, i])
    Q[:, i] ./= R[i, i]
  end
  return Q, R
end;
function MGS(X::Array{Float64,2})
 n, m = size(X)
  Q = Array{Float64,2}(undef, n, m)
  q = Vector{Float64}(undef, n)
 R = zeros(Float64, m, m)
  w = Vector{Float64}(undef, n)
 R[1, 1] = norm(X[:, 1])
  Q[:, 1] = X[:, 1] ./ R[1, 1]
  for i in 2:m
    w := X[:, i]
    for j in 1:i-1
     q = Q[:, j]
     R[j, i] = q'w
      w -= R[j, i] .* q
    end
    R[i, i] = norm(w)
    Q[:, i] = w ./ R[i, i]
  end
 return Q, R
end;
```

```
function CGS2_naive(X::Array{Float64,2})
    n, m = size(X)
    Q = Array{Float64,2}(undef, n, m)
    R = zeros(Float64, m, m)
    R[1, 1] = norm(X[:, 1])
    Q[:, 1] = X[:, 1] ./ R[1, 1]
    for i in 2:m
    Q[:, i] = X[:, i]
    R[1:i-1, i] .= Q[:, 1:i-1]'X[:, i] # creates temporary array => very slow
    Q[:, i] -= Q[:, 1:i-1] * R[1:i-1, i] # creates temporary array => very slow
```

```
r = Q[:, 1:i-1]'Q[:, i] # creates temporary array => very slow
    Q[:, i] = Q[:, 1:i-1] * r # creates temporary array => very slow
    R[i, i] = norm(Q[:, i])
    Q[:, i] ./= R[i, i]
  end
 return Q, R
end;
function CGS2(X::Array{Float64,2})
 n, m = size(X)
  Q = zeros(Float64, n, m)
 R = zeros(Float64, m, m)
 r = zeros(Float64, m)
  w = zeros(Float64, n)
 R[1, 1] = norm(X[:, 1])
  Q[:, 1] = X[:, 1] ./ R[1, 1]
  for i in 2:m
    w = X[:, i]
   r .= Q'w
    r[i:m] = 0.
   R[:, i] = r
    w -= Q * r
    r .= Q'w
    r[i:m] = 0.
    w -= Q * r
   R[i, i] = norm(w)
    Q[:, i] = w . / R[i, i]
  end
 return Q, R
end;
```

# Exercise #5: Compare runtime, loss of orthogonality and residual of CGS, MGS and CGS2

```
[20]: Q, R = @btime CGS_naive(A1);
Q, R = @btime CGS(A1);
@printf "||A - QR|| = %.2E, ||I - Q'Q|| = %.2E" norm(A1 - Q * R) norm(I - Q'Q)

55.181 ms (5985 allocations: 316.59 MiB)
14.985 ms (2806 allocations: 8.31 MiB)
||A - QR|| = 2.45E-15, ||I - Q'Q|| = 9.54E-08

[21]: Q, R = @btime CGS(A2);
@printf "||A - QR|| = %.2E, ||I - Q'Q|| = %.2E" norm(A2 - Q * R) norm(I - Q'Q)

14.345 ms (2806 allocations: 8.31 MiB)
||A - QR|| = 2.47E-15, ||I - Q'Q|| = 1.43E-05
```

```
[22]: Q, R = @btime MGS_naive(A1);
                          Q, R = Obtime MGS(A1);
                          Q_{P} = M - Q_{R} = M - Q_{R
                                140.893 ms (359807 allocations: 925.59 MiB)
                                82.462 ms (180315 allocations: 464.51 MiB)
                        ||A - QR|| = 3.81E-15, ||I - Q'Q|| = 1.35E-08
[23]: Q, R = Obtime MGS(A2);
                           Q_{P_{A}} Q_{P
                               73.142 ms (180315 allocations: 464.51 MiB)
                        ||A - QR|| = 3.85E-15, ||I - Q'Q|| = 1.47E-06
[24]: Q, R = Obtime CGS2_naive(A1);
                          Q, R = Obtime CGS2(A1);
                          Q_{P} ||A - Q_{R}|| = %.2E, ||I - Q'Q|| = %.2E'' norm(A1 - Q * R) norm(I - Q'Q)
                               110.824 ms (9965 allocations: 626.57 MiB)
                        ||A - QR|| = 3.30E-15, ||I - Q'Q|| = 5.73E-15 27.846 ms (4398 allocations:
                       11.69 MiB)
                        ||A - QR|| = 3.30E-15, ||I - Q'Q|| = 5.55E-15
[25]: Q, R = Obtime CGS2(A2);
                          Qrintf "|A - QR| = %.2E, |I - Q'Q| = %.2E" norm(A2 - Q * R) norm(I - Q'Q)
                                28.367 ms (4398 allocations: 11.69 MiB)
                        ||A - QR|| = 3.33E-15, ||I - Q'Q|| = 5.36E-15
```

## Exercise #6: Implement Golub-Kahan bidiagonalization and verify matrix transformation

```
[26]: function bidiagonalization(A, r0, k)
        m, n = size(A)
        U = zeros(Float64, m, k + 1)
        V = zeros(Float64, n, k + 1)
        beta = zeros(Float64, k + 1)
        alpha = zeros(Float64, k + 1)
        U[:, 1] = r0
        beta[1] = norm(U[:,1])
        U[:, 1] = U[:, 1] ./ beta[1]
        V[:, 1] = A'U[:, 1]
        alpha[1] = norm(V[:, 1])
        V[:, 1] = V[:, 1] ./ alpha[1]
        for i = 1:k
          U[:, i + 1] = A * V[:, i] - alpha[i] * U[:, i]
          beta[i + 1] = norm(U[:, i + 1])
          U[:, i + 1] = U[:, i + 1] / beta[i + 1]
```

```
V[:, i + 1] = A'U[:, i + 1] - beta[i + 1] * V[:, i]
          alpha[i + 1] = norm(V[:, i + 1])
          V[:, i + 1] = V[:, i + 1] / alpha[i + 1]
       return U, V[:, 1:k], alpha[1:k], beta
      end;
[27]: Random.seed!(3)
      m = 100 000; n = 200;
      A = sprand(Float64, m, n, .4);
      b = rand(m);
[28]: k = 5;
      U, V, alpha, beta = bidiagonalization(A, rand(m), k);
      B = spdiagm(k + 1, k, 0 => alpha, -1 => beta[2:k+1]);
      norm(U'A*V - B)
[28]: 6.415087381394998
[29]: U'A*V
[29]: 6×5 Matrix{Float64}:
      773.996
                       8.41039e-11
                                     1.57414e-7
                                                  0.000298512
                                                                0.589457
       457.727
                       4.65152
                                     9.30947e-8
                                                  0.00017654
                                                                0.348604
        9.09368e-10 96.5391
                                     4.41971
                                                  9.91893e-8
                                                                0.000195861
        1.70404e-6
                      4.54171e-9
                                    96.5037
                                                  4.36742
                                                                1.04521e-7
        0.00322698
                       8.59641e-6
                                     4.58986e-9 96.6373
                                                                4.1883
        6.37841
                       0.0169915
                                     9.07075e-6
                                                  4.78334e-9
                                                               96.5428
[30]: B
[30]: 6×5 SparseMatrixCSC{Float64, Int64} with 10 stored entries:
       773.996
       457.727
                 4.65152
               96.5391
                          4.41971
                         96.5037
                                    4.36742
                                  96.6373
                                              4.1883
                                            96.5428
[31]: norm(I - U'U)
[31]: 0.01003147391463673
[32]: norm(I - V'V)
[32]: 0.0010770355772659224
```

#### Exercise #7: Implement and test LSQR

```
[33]: function LSQR(A, b, x0, k, tol)
       A_F = sqrt(sum(A.nzval.^2))
        m, n = size(A)
        U = zeros(Float64, m, k + 1)
        V = zeros(Float64, n, k)
        B = spdiagm(k + 1, k, 0 = zeros(Float64, k), -1 = zeros(Float64, k))
        U[:, 1] = b - A * x0
        beta1 = norm(U[:,1])
        U[:, 1] = U[:, 1] ./ beta1
        V[:, 1] = A'U[:, 1]
        B[1, 1] = norm(V[:, 1])
        V[:, 1] = V[:, 1] / B[1, 1]
        beta1_x_e1 = zeros(Float64, k + 1); beta1_x_e1[1] = beta1
        i = 0
        err = 1.
        yi = 1.
        while (err > tol && i < k)
          U[:, i + 1] = A * V[:, i] - B[i, i] * U[:, i]
          B[i + 1, i] = norm(U[:, i + 1])
          U[:, i + 1] = U[:, i + 1] / B[i + 1, i]
          V[:, i + 1] = A'U[:, i + 1] - B[i + 1, i] * V[:, i]
          B[i + 1, i + 1] = norm(V[:, i + 1])
          V[:, i + 1] = V[:, i + 1] / B[i + 1, i + 1]
          yi = B[1:i+1, 1:i] \setminus beta1_x_e1[1:i+1]
          ti = beta1_x_e1[1:i+1] - B[1:i+1, 1:i] * yi # //ti// = //ri//
          si = B[1:i+1, 1:i+1]'ti
                                                        \# //si// = //A'ri//
          err = norm(si) / (A F * norm(ti))
          @printf "i = %i, ||A'ri||/(||A||.||ri||) = %.2E\n" i err
        return x0 + V[:, 1:i] * yi
      end;
[34]: x = LSQR(A, b, rand(n), 100, 1e-5);
      norm(b - A * x)
     i = 1, ||A'ri||/(||A||.||ri||) = 5.75E-02
     i = 2, ||A'ri||/(||A||.||ri||) = 1.07E-02
     i = 3, ||A'ri||/(||A||.||ri||) = 4.53E-04
     i = 4, ||A'ri||/(||A||.||ri||) = 2.17E-05
     i = 5, ||A'ri||/(||A||.||ri||) = 1.07E-06
[34]: 92.84273159426289
[35]: x = A \setminus b;
      norm(A * x - b)
```

### [35]: 92.84273158157164