

# PracticeSession11

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## Numerical Linear Algebra for Computational Science and Information Engineering

### Arnoldi and Lanczos Procedures

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```
[1]: using LinearAlgebra, Plots, Printf, Latexify, LaTeXStrings, BenchmarkTools, LinearAlgebra.jl
      ↪ ArnoldiMethod, SparseArrays
      using MatrixMarket: mmread
```

### Exercise #1: Implement MGS and CGS2-based Arnoldi

```
[2]: function MGS_arnoldi(A, q1::Vector{Float64}, k::Int)
      n, _ = size(A)
      Q = zeros(Float64, (n, k + 1))
      q = zeros(Float64, n)
      H = zeros(Float64, (k + 1, k))
      w = zeros(Float64, n)
      Q[:, 1] = q1 ./ norm(q1)
      for j in 1:k
          w .= A * Q[:, j]
          for i in 1:j
              q .= Q[:, i]
              H[i, j] = q'w
              w -= H[i, j] .* q
          end
          H[j + 1, j] = norm(w)
          Q[:, j + 1] = w ./ H[j + 1, j]
      end
      return Q, H
end;
```

```
[3]: function CGS2_arnoldi(A, q1::Vector{Float64}, k::Int)
      n, _ = size(A)
      Q = zeros(Float64, (n, k + 1))
      H = zeros(Float64, (k + 1, k))
      h = zeros(Float64, k + 1)
```

```

w = zeros(Float64, n)
Q[:, 1] = q1 ./ norm(q1)
for j in 1:k
    w .= A * Q[:, j]
    h .= Q'w
    h[j+1:k+1] .= 0.
    H[:, j] = h
    w -= Q * h
    h .= Q'w
    h[j+1:k+1] .= 0.
    w -= Q * h
    H[j + 1, j] = norm(w)
    Q[:, j + 1] = w ./ H[j + 1, j]
end
return Q, H
end;

```

## Exercise #2: Benchmark Arnoldi procedures

```

[4]: matrix_folder = "/home/venkovic/Dropbox/Git/matrix-market/";
A = mmread(matrix_folder * "G3_circuit.mtx");
n, _ = size(A);

```

```

[5]: k = 100;

```

```

[6]: Q, H = @time MGS_arnoldi(A, rand(n), k);
@printf "||Qjp1 * A * Qj - H|| = %.2E, ||A * Qj - Qjp1 * H|| = %.2E, ||I - Q'Q|| = %.2E" norm(Q'A * Q[:, 1:k] - H) norm(A * Q[:, 1:k] - Q * H) norm(I - Q'Q)

```

69.157852 seconds (1.03 M allocations: 183.798 GiB, 7.47% gc time, 0.79% compilation time)  
||Qjp1 \* A \* Qj - H|| = 3.06E-07, ||A \* Qj - Qjp1 \* H|| = 5.49E-11, ||I - Q'Q|| = 2.19E-11

```

[7]: Q, H = @time CGS2_arnoldi(A, rand(n), k);
@printf "||Qjp1 * A * Qj - H|| = %.2E, ||A * Qj - Qjp1 * H|| = %.2E, ||I - Q'Q|| = %.2E" norm(Q'A * Q[:, 1:k] - H) norm(A * Q[:, 1:k] - Q * H) norm(I - Q'Q)

```

17.489222 seconds (788.68 k allocations: 9.537 GiB, 2.74% gc time, 1.19% compilation time)  
||Qjp1 \* A \* Qj - H|| = 3.19E-10, ||A \* Qj - Qjp1 \* H|| = 1.03E-10, ||I - Q'Q|| = 1.54E-14

### Exercise #3: Implement Rayleigh-Ritz procedure with CGS2-based Arnoldi

```
[8]: function RR_CGS2_arnoldi(A, q1::Vector{Float64}, k::Int, nev::Int, tol::Float64)
    n, _ = size(A)
    Q = zeros(Float64, (n, k + 1))
    H = zeros(Float64, (k + 1, k))
    h = zeros(Float64, k + 1)
    w = zeros(Float64, n)
    Q[:, 1] = q1 ./ norm(q1)
    j = 0
    res = 1.; vals = nothing; vecs = nothing; order = nothing
    while (maximum(res) > tol && j < k)
        j += 1
        w .= A * Q[:, j]
        h .= Q'w
        h[j+1:k+1] .= 0.
        H[:, j] = h
        w -= Q * h
        h .= Q'w
        h[j+1:k+1] .= 0.
        w -= Q * h
        H[j + 1, j] = norm(w)
        Q[:, j + 1] = w ./ H[j + 1, j]
        vals, vecs = eigen(H[1:j, 1:j], sortby=norm)
        order = (j:-1:j-min(nev,j)+1)
        res = norm(H[j + 1, j]) .* norm.(vecs[j, order]) ./ norm.(vals[order])
        println(res)
    end
    return res, vals[order], Q[:, 1:j] * vecs[:, order]
end;
```

```
[9]: A = mmread(matrix_folder * "nxp1.mtx");
    n, _ = size(A);
```

```
[10]: k = 100;
    nev = 5;
    tol = 1e-6;
    res, vals, Y = RR_CGS2_arnoldi(A, rand(n), k, nev, tol);
```

```
[7.122190536983693]
[0.8213522929785088, 9.132070839382395]
[0.5090906451152992, 0.9879623558688576, 9.85342639352183]
[0.2273285199551234, 0.4130076592013465, 0.8011141775928895, 7.287252375293572]
[0.0696241098782475, 0.2601789558053935, 0.606765853883062, 1.07063419974055,
7.854856070851897]
[0.02013586829794183, 0.1780901942406374, 0.27429748430277373,
0.524671225477858, 1.3501215708298435]
[0.005564758513671639, 0.11108444163147926, 0.2112494665794819,
```

0.4192124328680065, 0.5246420362943479]  
 [0.003241196162871559, 0.21812661373313652, 0.32094412867700595,  
 0.2957351880150637, 0.49040313059309226]  
 [0.001529257320021997, 0.13255933323165336, 0.07110862903214481,  
 0.12807679626255883, 0.25674920629979]  
 [0.00047570169093799636, 0.05096215691801789, 0.044388988086093914,  
 0.1735011136480694, 0.27515939270303824]  
 [9.060420082827789e-5, 0.013461710384683696, 0.025131351611863285,  
 0.12178200953833454, 0.0966774419378679]  
 [2.480720137416568e-5, 0.005142123151920981, 0.01982634357677782,  
 0.11098419590256546, 0.13133565736668845]  
 [5.523307124158734e-6, 0.0016440902793090969, 0.016493978884688204,  
 0.09718203495735295, 0.13973087395052017]  
 [1.4986916828563523e-6, 0.0006311171095354178, 0.015915255740037,  
 0.08575982027770794, 0.11707021704148865]  
 [3.764498234940891e-7, 0.00023183567243255767, 0.020422509429696492,  
 0.08037106485218173, 0.10939179995826011]  
 [7.017458617381005e-8, 6.110851028095134e-5, 0.018413628741781842,  
 0.04316979129305967, 0.06050868476768572]  
 [1.0512390392638043e-8, 1.211527908048221e-5, 0.006946285302789791,  
 0.014333876246300108, 0.024058549793084735]  
 [2.354108594139101e-9, 3.6600643158732877e-6, 0.003671771359246678,  
 0.0077562391051702005, 0.016882702444002536]  
 [6.772883877146847e-10, 1.5120649861339995e-6, 0.003386290481252761,  
 0.007720414556915467, 0.031269097670277544]  
 [1.8611029484504923e-10, 6.247993008640811e-7, 0.005497030985714999,  
 0.01656901796125485, 0.15207798140046963]  
 [3.645145537199201e-11, 1.7303266145778361e-7, 0.008946728006890696,  
 0.05381346778173956, 0.03902560454797512]  
 [6.881037592943361e-12, 4.451834970236423e-8, 0.008331493380073716,  
 0.02661361333101909, 0.009855200932608364]  
 [1.1500413357947851e-12, 1.0001576401107346e-8, 0.00397706860288316,  
 0.01020989503348323, 0.0036333560284036175]  
 [2.0802981025750184e-13, 2.4227908450018322e-9, 0.0016921966230976095,  
 0.004233249348859367, 0.0015518718670809776]  
 [4.0493449250762256e-14, 6.353061086584785e-10, 0.0007742539740376854,  
 0.0019504253568809239, 0.0007444723553651325]  
 [1.2566535073591226e-14, 2.793958356037041e-10, 0.0007041471748913218,  
 0.0018074784581070527, 0.0007348496655812858]  
 [3.2145499041345e-15, 1.0779969238873965e-10, 0.0010565607315571328,  
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 [6.230203109232408e-16, 2.943625056664814e-11, 0.0012994748355210813,  
 0.004397026721698786, 0.041354370318295836]  
 [9.654609131173383e-17, 6.10651049952696e-12, 0.0006657496140699028,  
 0.002726291323704814, 0.022289496849780755]  
 [2.2289940131143213e-17, 1.8893986224027858e-12, 0.00036995892931629296,  
 0.001597262389595893, 0.011891870428837908]  
 [6.997419708231792e-18, 8.73169105656125e-13, 0.00043555147370195776,

```

0.0019867880604861757, 0.014354485000256309]
[1.6863515460075304e-18, 3.140161774215281e-13, 0.0008326251688446404,
0.004748722286229888, 0.030452863700431425]
[3.310248804890951e-19, 8.556952387350583e-14, 0.0017289188455382953,
0.03203541590417306, 0.021844211543650526]
[5.868002751681107e-20, 2.0509988193647936e-14, 0.0026317134677900497,
0.0176827177657614, 0.0034149972989214426]
[9.74510499481637e-21, 4.542180639048697e-15, 0.0016796242294342418,
0.006585091513860168, 0.0011531454796306505]
[1.6600163575652082e-21, 1.0365354156961066e-15, 0.0007079002836209883,
0.0025068322088831526, 0.0004395343738557693]
[2.9747437650666357e-22, 2.4739606026909816e-16, 0.000289665815349205,
0.0010109759258506996, 0.00017907403126149585]
[4.457735897719192e-23, 4.893932362650456e-17, 9.727240679234407e-5,
0.0003392042369315683, 6.077076361834172e-5]
[6.202783724731967e-24, 8.817321485213572e-18, 2.726756738364179e-5,
9.520051374623115e-5, 1.7215010964657158e-5]
[6.604752997998509e-25, 1.995382893899237e-18, 9.999816107103177e-6,
3.4965188585013424e-5, 6.384525253841525e-6]
[5.528475003946488e-25, 4.374350244214967e-19, 3.6673488124526587e-6,
1.2845242449094228e-5, 2.3715066183115723e-6]
[3.2011261912621844e-26, 1.0182749071460517e-19, 1.4175345260451094e-6,
4.973554124766851e-6, 9.283510666730071e-7]
[3.853236020826537e-26, 2.53662947155469e-20, 5.415554922010912e-7,
1.903501965060257e-6, 3.594031755945758e-7]
[9.961820465860394e-28, 5.0642212203567736e-21, 1.9752541246606059e-7,
6.954738623551596e-7, 1.3277042703436866e-7]

```

```

[11]: res2 = [norm(A * Y[:, i] - vals[i] .* Y[:, i]) / norm(vals[i]) for i in 1:nev];
maximum(res - res2)

```

```

[11]: -2.7830326273224106e-19

```

```

[12]: decomp, hist = partialschur(A, nev=nev);
vals2, Y2 = partialeigen(decomp);

```

```

[13]: maximum(abs.(vals2[end:-1:1] .- vals))

```

```

[13]: 2.566480361565482e-10

```

```

[14]: norm(abs.(Y'Y2[:, end:-1:1]) - I)

```

```

[14]: 5.285318735527176e-10

```

```

[15]: vals

```

```

[15]: 5-element Vector{Float64}:
 414.7385747346634

```

341.53916763358933  
 257.3852366214957  
 257.18132297539614  
 255.8853137892908

#### Exercise #4: Implement harmonic Ritz procedure with CGS2-based Arnoldi

```
[16]: function HR_CGS2_arnoldi(A, q1::Vector{Float64}, k::Int, nev::Int, sigma::
    ↪ComplexF64, tol::Float64)
    n, _ = size(A)
    Q = zeros(Float64, (n, k + 1))
    H = zeros(Float64, (k + 1, k))
    h = zeros(Float64, k + 1)
    w = zeros(Float64, n)
    Q[:, 1] = q1 ./ norm(q1)
    j = 0
    res = 1.; rho = nothing; vecs = nothing
    while (maximum(res) > tol && j < k)
        j += 1
        w .= A * Q[:, j]
        h .= Q'w
        h[j+1:k+1] .= 0.
        H[:, j] = h
        w -= Q * h
        h .= Q'w
        h[j+1:k+1] .= 0.
        w -= Q * h
        H[j + 1, j] = norm(w)
        Q[:, j + 1] = w ./ H[j + 1, j]
        e_j = zeros(Float64, j); e_j[j] = 1.
        f = (H[1:j, 1:j] - sigma * I)' \ e_j
        G = H[1:j, 1:j] + norm(H[j + 1, j])^2 .* f * e_j'
        vals, vecs = eigen(G)
        order = sortperm(norm.(vals .- sigma))[1:minimum([j, nev])]
        vals = vals[order]
        vecs = vecs[:, order]
        rho = [vals[i] - norm(H[j + 1, j])^2 * vecs[:, i]'f * vecs[j, i] for i in 1:
    ↪minimum([j, nev])]
        res = sqrt.(real.((vals .- rho) .* conj.(rho .- sigma)))
        res ./= norm.(rho)
        #hres = (vals .- rho) .* conj.(vals .- sigma)
        println(res)
    end
    return res, rho, Q[:, 1:j] * vecs
end;
```

```
[17]: k = 500
      nev = 2;
      sigma = 150. + 0im;
      res, vals, Y = HR_CGS2_arnoldi(A, rand(n), k, nev, sigma, tol);
```

```
[7.1533009469765005]
[0.8347931699754206, 6.965511864238601]
[0.7447323401602826, 11.615621258471972]
[0.7446611957425694, 12.056859813018207]
[0.4692006024418052, 0.2463101153680702]
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[0.10711384644426265, 0.18744545315384703]
[0.10533840544451503, 0.18673476965799582]
[0.09014495867313536, 0.12925256634201995]
[0.08239838565996903, 0.1311511535107435]
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[0.06917905782274152, 0.1026973614329002]
[0.07000517057626393, 0.08594696905715747]
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[0.03393634720731764, 0.04195784105041194]
[0.03388804807793444, 0.04195620884531937]
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[0.027981847061368467, 0.03789637399931903]
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[0.02234300216265498, 0.03271894128915769]
[0.018364113857962307, 0.02929788824551029]
[0.017942590904929105, 0.029433714681066696]
[0.016827696886601948, 0.02685762872163033]
[0.014813301511314476, 0.025118617499353804]
[0.01461573941687391, 0.02538322127887674]
```

[0.014227245755995288, 0.023440271535246877]  
[0.013089904465224138, 0.022871640290794915]  
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[0.012010257291139834, 0.021881342411698094]  
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```

```

[18]: res2 = [norm(A * Y[:, i] - vals[i] .* Y[:, i]) / norm(vals[i]) for i in 1:nev];
      maximum(res - res2)

```

```

[18]: 4.581184905592847e-14

```

```

[19]: vals

```

```

[19]: 2-element Vector{ComplexF64}:
      151.07427423364803 - 6.242451922324095e-15im
      151.37728530092386 - 7.396799549638819e-15im

```

```

[20]: res

```

```

[20]: 2-element Vector{Float64}:
      9.525835318490645e-8
      6.913572547902072e-7

```

## Exercise #5: Implement the Lanczos procedure

```

[21]: function lanczos(A, q1::Vector{Float64}, k::Int)
      n, _ = size(A)
      Q = zeros(Float64, (n, k + 1))
      v = zeros(Float64, n)
      T = zeros(Float64, k + 1, k + 1)

```

```

Q[:, 1] = q1 ./ norm(q1)
for j in 1:k
    v = A * Q[:, j]
    T[j, j] = Q[:, j]'v
    v = v - T[j, j] * Q[:, j]
    if (j > 1)
        v -= T[j, j - 1] * Q[:, j - 1]
    end
    T[j + 1, j] = norm(v); T[j, j + 1] = T[j + 1, j]
    Q[:, j + 1] = v ./ T[j + 1, j]
end
return Q, T[1:k+1, 1:k]
end;

```

```

[22]: A = mmread(matrix_folder * "Kuu.mtx");
n, _ = size(A);

```

```

[23]: k = 100;

```

```

[24]: Q, T = @time lanczos(A, rand(n), k);
@printf "| |Qjp1 * A * Qj - T| | = %.2E, | |A * Qj - Qjp1 * T| | = %.2E, | |I - Q'Q| | = %.2E" norm(Q'A * Q[:, 1:k] - T) norm(A * Q[:, 1:k] - Q * T) norm(I - Q'Q)

```

0.162612 seconds (83.75 k allocations: 63.608 MiB, 19.92% gc time, 67.10% compilation time)

| |Qjp1 \* A \* Qj - T| | = 4.00E-09, | |A \* Qj - Qjp1 \* T| | = 2.44E-14, | |I - Q'Q| | = 8.05E-11

## Exercise #6: Implement Rayleigh-Ritz procedure with Lanczos

```

[25]: function RR_lanczos(A, q1::Vector{Float64}, k::Int, nev::Int, tol::Float64)
    n, _ = size(A)
    Q = zeros(Float64, (n, k + 1))
    v = zeros(Float64, n)
    T = zeros(Float64, k + 1, k + 1)
    vals = zeros(Float64, nev, k)
    Q[:, 1] = q1 ./ norm(q1)
    j = 0
    res = 1.; vecs = nothing; order = nothing
    while (maximum(res) > tol && j < k)
        j += 1
        v = A * Q[:, j]
        T[j, j] = Q[:, j]'v
        v = v - T[j, j] * Q[:, j]
        if (j > 1)
            v -= T[j, j - 1] * Q[:, j - 1]
        end
    end
end

```

```

    T[j + 1, j] = norm(v); T[j, j + 1] = T[j + 1, j]
    Q[:, j + 1] = v ./ T[j + 1, j]
    _vals, vecs = eigen(T[1:j, 1:j], sortby=norm)
    order = (j:-1:j-min(nev,j)+1)
    vals[1:minimum([j, nev]), j] = _vals[order]
    res = norm(T[j + 1, j]) .* norm.(vecs[j, order]) ./ norm.(_vals[order])
    println(res)
end
return res, vals[:, 1:j], Q[:, 1:j] * vecs[:, order]
end;

```

```

[26]: k = 500;
nev = 5;
res, vals, Y = RR_lanczos(A, rand(n), k, nev, tol);

```

```

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```

```
[27]: res2 = [norm(A * Y[:, i] - vals[i, end] .* Y[:, i]) / norm(vals[i, end]) for i =
    ↪in 1:nev];
maximum(res - res2)
```

```
[27]: 1.1672503134646086e-17
```

```
[28]: vals[:, end]
```

```
[28]: 5-element Vector{Float64}:
 54.082055996412535
 53.98165804506269
 53.815496452830146
 53.720402051506426
 53.622541454743214
```

## Exercise #7: Implement harmonic Ritz procedure with Lanczos

```
[29]: function HR_lanczos(A, q1::Vector{Float64}, k::Int, nev::Int, sigma::Float64,
    ↪tol::Float64)
    n, _ = size(A)
    Q = zeros(Float64, (n, k + 1))
    v = zeros(Float64, n)
    T = zeros(Float64, k + 1, k + 1)
    rhos = zeros(ComplexF64, nev, k)
    Q[:, 1] = q1 ./ norm(q1)
    j = 0
    res = 1.; vecs = nothing; order = nothing
    while (maximum(res) > tol && j < k)
        j += 1
        v = A * Q[:, j]
        T[j, j] = Q[:, j]'v
        v = v - T[j, j] * Q[:, j]
        if (j > 1)
            v -= T[j, j - 1] * Q[:, j - 1]
        end
        T[j + 1, j] = norm(v); T[j, j + 1] = T[j + 1, j]
        Q[:, j + 1] = v ./ T[j + 1, j]
        e_j = zeros(Float64, j); e_j[j] = 1.
        f = (T[1:j, 1:j] - sigma * I) \ e_j
        G = T[1:j, 1:j] + T[j + 1, j]^2 .* f * e_j'
        vals, vecs = eigen(G)
```

```

    order = sortperm(norm.(vals .- sigma))[1:minimum([j, nev])]
    vals = vals[order]
    vecs = vecs[:, order]
    rho = [vals[i] - T[j + 1, j]^2 * vecs[:, i]'f * vecs[j, i] for i in 1:
    ↪minimum([j, nev])]
    res = sqrt.(real.((vals .- rho) .* conj.(rho .- sigma)))
    res ./= norm.(rho)
    rhos[1:minimum([j, nev]), j] = rho
    println(res)
end
return res, rhos[:, 1:j], Q[:, 1:j] * vecs
end;

```

```

[30]: k = 1_000;
nev = 2;
sigma = 25.;
res, vals, Y = HR_lanczos(A, rand(n), k, nev, sigma, tol);

```

```

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```

[31]: res2 = [norm(A * Y[:, i] - vals[i, end] .* Y[:, i]) / norm(vals[i, end]) for i_
↳in 1:nev];
maximum(res - res2)

```

```

[31]: 3.693715865398135e-15

```

```

[32]: vals[:, end]

```

```

[32]: 2-element Vector{ComplexF64}:
 25.00555991429552 + 0.0im
 25.061552975162282 + 0.0im

```

```

[33]: Y

```

```

[33]: 7102×2 Matrix{Float64}:
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-0.00334998 -0.00421567
-0.00610707 -0.010005
 0.00360302  0.00390971
 0.0101474  0.0159739
 0.00257309  0.00371054
-0.00166761 -0.00151604
-0.00857561 -0.010363
-0.012858   -0.0192621
 0.00519499  0.00561935
 0.0140195   0.0192926
 0.00487764  0.00556101
 0.000283372 0.00149261

 4.84202e-6  6.19084e-6
-7.45918e-7 -1.12588e-6
-4.7724e-6  -6.39985e-6
-1.07311e-6 -1.13519e-6
 3.29972e-7  2.90996e-7
 9.14683e-7  1.04169e-6
 2.67948e-6  4.05669e-6
 1.15438e-8  -3.46597e-8

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-2.61874e-6	-3.68752e-6
-1.0549e-6	-1.37632e-6
1.96574e-7	2.4588e-7
3.83117e-7	4.99403e-7