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Overview

- 1. Sparse matrix representation.
 - COOrdinate (COO) format
 - Compressed Sparse Column/Row (CSC/CSR) format
- 2. Solving the dominant eigenvalue problem.
 - Symmetric Lanczos process
 - Anoldi process

Sparse Matrices

```
1 using LinearAlgebra, SparseArrays
```

Recall that the elementary elimination matrix in Gaussian elimination has the following form.

$$M_k = egin{pmatrix} 1 & \dots & 0 & 0 & 0 & \dots & 0 \ dots & \ddots & dots & dots & \ddots & dots \ 0 & \dots & 1 & 0 & 0 & \dots & 0 \ 0 & \dots & 0 & 1 & 0 & \dots & 0 \ 0 & \dots & 0 & -m_{k+1} & 1 & \dots & 0 \ dots & \ddots & dots & dots & \ddots & dots \ 0 & \dots & 0 & -m_n & 0 & \dots & 1 \end{pmatrix}$$

where $m_i = a_i/a_k$

The following cell is copied from notebook: 4.linearequation.jl

elementary_elimination_matrix (generic function with 1 method)

```
function elementary_elimination_matrix(A::AbstractMatrix{T}, k::Int) where T
n = size(A, 1)
@assert size(A, 2) == n
# create Elementary Elimination Matrices
M = Matrix{Float64}(I, n, n)
for i=k+1:n
M[i, k] = -A[i, k] ./ A[k, k]
end
return M
end
```

```
some_random_matrix = 5×5 reshape(::UnitRange{Int64}, 5, 5) with eltype Int64:
                         6 11 16 21
                         7 12 17
                        8 13 18 23
                              19 24
                       10 15 20 25
 1 some_random_matrix = reshape(1:25, 5, 5)
demo_matrix = 5×5 Matrix{Float64}:
                                  0.0 0.0
              1.0 0.0
                         0.0
              0.0
                  1.0
                         0.0
                                  0.0 0.0
                  0.0
                        1.0
                                  0.0
                                       0.0
              0.0 \quad 0.0 \quad -1.07692
                                 1.0
                                       0.0
              0.0 0.0 -1.15385 0.0 1.0
 1 demo_matrix = elementary_elimination_matrix(some_random_matrix, 3)
```

This representation requires storing n^2 elements, which is very memory inefficient since it has only 2n - k nonzero elements.

Let $A \in \mathbb{R}^{m \times n}$ be a sparse matrix, and $\mathbf{nnz}(A) \ll mn$ be the number of nonzero elements in A. Is there a universal matrix type that stores such sparse matrices efficiently?

The answer is yes.

COOrdinate (COO) format

The coordinate format means storing nonzero matrix elements into triples

```
egin{aligned} (i_1,j_1,v_1) \ (i_2,j_2,v_2) \ dots \ (i_k,j_k,v_k) \end{aligned}
```

Quiz: How many bytes are required to store the matrix demo_matrix in the COO format?

```
struct COOMatrix{T} <: AbstractArray{T, 2}  # Julia does not have a COO data type
rowval::Vector{Int}  # row indices
colval::Vector{Int}  # column indices
nzval::Vector{T}  # values
m::Int  # number of rows
n::Int  # number of columns
end</pre>
```

We need to implement the AbstractArray interfaces.

```
1 Base.size(coo::COOMatrix{T}) where T = (coo.m, coo.n)
```

```
1 Base.size(coo::COOMatrix{T}, i::Int) where T = getindex((coo.m, coo.n), i)
```

Indexing a COO matrix

Element indexing requires O(nnz(A)) time.

```
function Base.getindex(coo::COOMatrix{T}, i::Integer, j::Integer) where T
v = zero(T)
for (i2, j2, v2) in zip(coo.rowval, coo.colval, coo.nzval)
if i == i2 && j == j2
v += v2 # accumulate the value, since repeated indices are allowed.
end
end
return v
end
```

```
coo_matrix = 5×5 COOMatrix{Float64}:
                                    0.0
             1.0 0.0
                      0.0
                                0.0
             0.0 1.0
                       0.0
                                0.0 0.0
             0.0 0.0
                       1.0
                                0.0
                                    0.0
             0.0 0.0 -1.07692 1.0
                                    0.0
             0.0 0.0 -1.15385 0.0 1.0
 1 coo_matrix = COOMatrix([1, 2, 3, 4, 5, 4, 5], [1, 2, 3, 4, 5, 3, 3], [1, 1, 1, 1, 1,
   demo_matrix[4,3], demo_matrix[5, 3]], 5, 5)
```

```
1 # uncomment to show the result
2 sizeof(coo_matrix)
```

Multiplying two COO matrices

In the following example, we compute coo_matrix * coo_matrix.

```
6
       for (i, j, v) in zip(A.rowval, A.colval, A.nzval)
           for (i2, j2, v2) in zip(B.rowval, B.colval, B.nzval)
 8
               if j == i2
 9
                   push!(rowval, i)
10
                   push!(colval, j2)
                   push!(nzval, v * v2)
11
12
               end
13
           end
14
       end
15
       return COOMatrix(rowval, colval, nzval, size(A, 1), size(B, 2))
16 end
5×5 COOMatrix{Float64}:
1.0 0.0
          0.0
                    0.0
                         0.0
0.0 1.0
           0.0
                    0.0 0.0
0.0 0.0
          1.0
                    0.0 0.0
0.0 0.0 -2.15385
                    1.0 0.0
0.0 0.0 -2.30769 0.0 1.0
 1 coo_matrix * coo_matrix
5×5 Matrix{Float64}:
1.0 0.0
          0.0
                    0.0 0.0
0.0 1.0
           0.0
                    0.0 0.0
0.0 0.0
           1.0
                    0.0
                         0.0
0.0 0.0 -2.15385
                    1.0
                         0.0
0.0 0.0 -2.30769 0.0 1.0
 1 demo_matrix ^ 2
```

1 function Base.:(*)(A::COOMatrix{T1}, B::COOMatrix{T2}) where {T1, T2}

Qassert size(A, 2) == size(B, 1)

nzval = promote_type(T1, T2)[]

rowval = Int[]
colval = Int[]

Yep!

3

45

- Quiz 1: What is the time complexity of COO matrix setindex! (A[i, j] += v)?
- Quiz 2: What is the time complexity of COO matrix multiplication?

Compressed Sparse Column (CSC) format

A CSC format sparse matrix can be constructed with the SparseArrays.sparse function

```
(:m, :n, :colptr, :rowval, :nzval)
1 fieldnames(csc_matrix |> typeof)
```

The m, n, rowval and nzval have the same meaning as those in the COO format. colptr is a integer vector of size n+1, the element of which points to the elements in rowval and nzval. Given a matrix $A \in \mathbb{R}^{m \times n}$ in the CSC format, the j-th column of A is defined as

```
A[rowval[colptr[j]:colptr[j+1]-1], j] := nzval[colptr[j]:colptr[j+1]-1]
```

```
SparseArrays.SparseVector{Float64, Int64}: [0.0, 0.0, 1.0, -1.07692, -1.15385]

1 csc_matrix[:, 3]
```

The row indices of nonzero elements in the 3rd column.

```
rows3 = [3, 4, 5]
1 rows3 = csc_matrix.rowval[csc_matrix.colptr[3]:csc_matrix.colptr[4]-1]

[3, 4, 5]
1 # or equivalently in Julia, we can use 'nzrange'
2 csc_matrix.rowval[nzrange(csc_matrix, 3)]
```

The values of nonzero elements in the 3rd column.

Indexing a CSC matrix

The number of operations required to index an element in the j-th column of a CSC matrix is linear to the nonzero elements in the j-th column.

my_getindex (generic function with 1 method)

```
# I do not want to overwrite 'Base.getindex'
function my_getindex(A::SparseMatrixCSC{T}, i::Int, j::Int) where T

for k in nzrange(A, j)

if A.rowval[k] == i

return A.nzval[k]

end

end

return zero(T)

end
```

```
1 my_getindex(csc_matrix, 4, 3)
```

1.0

1 csc_matrix^2

-2.15385 1.0 -2.30769 •

Multiplying two CSC matrices

Multiplying two CSC matrices is much faster than multiplying two COO matrices.

```
my_matmul (generic function with 1 method)
 1 function my_matmul(A::SparseMatrixCSC{T1}, B::SparseMatrixCSC{T2}) where {T1, T2}
       T = promote_type(T1, T2)
 3
       Qassert size(A, 2) == size(B, 1)
       rowval, colval, nzval = Int[], Int[], T[]
       for j2 in 1:size(B, 2) # enumerate the columns of B
           for k2 in nzrange(B, j2) # enumerate the rows of B
 6
               v2 = B.nzval[k2]
               for k1 in nzrange(A, B.rowval[k2]) # enumerate the rows of A
 9
                    push!(rowval, A.rowval[k1])
                    push!(colval, j2)
10
                    push!(nzval, A.nzval[k1] * v2)
11
12
               end
13
           end
14
       end
15
       return sparse(rowval, colval, nzval, size(A, 1), size(B, 2))
16 end
5×5 SparseMatrixCSC{Float64, Int64} with 7 stored entries:
 1.0
     1.0
            1.0
           -2.15385 1.0
           -2.30769
                          1.0
 1 my_matmul(csc_matrix, csc_matrix)
5×5 SparseMatrixCSC{Float64, Int64} with 7 stored entries:
 1.0
      1.0
```

Quiz: What is the time complexity of CSC matrix setindex! (A[i, j] = v)?

Large sparse eigenvalue problem

Dominant eigenvalue problem

One can use the power method to compute dominant eigenvalues (one having the largest absolute value) of a matrix.

power_method (generic function with 1 method)

```
function power_method(A::AbstractMatrix{T}, n::Int) where T
n = size(A, 2)
x = normalize!(randn(n))
for i=1:n
x = A * x
normalize!(x)
end
return x' * A * x', x
end
end
```

Since computing matrix-vector multiplication of CSC sparse matrix is fast, the power method is a convenient method to obtain the largest eigen value of a sparse matrix.

The rate of convergence is dedicated by $|\lambda_2/\lambda_1|^k$.

By inverting the sign, $A \rightarrow -A$, we can use the same method to obtain the smallest eigenvalue.

The symmetric Lanczos process

Let $A \in \mathbb{R}^{n \times n}$ be a large symmetric sparse matrix, the Lanczos process can be used to obtain its largest/smallest eigenvalue, with faster convergence speed comparing with the power method.

The Krylov subspace

A Krylov subspace of size $m{k}$ with initial vector $m{q_1}$ is defined by

$$\mathcal{K}(A, q_1, k) = \mathrm{span}\{q_1, Aq_1, A^2q_1, \dots, A^{k-1}q_1\}$$

The Julia package KrylovKit.jl contains many Krylov space based algorithms.

KrylovKit.jl accepts general functions or callable objects as linear maps, and general Julia objects with vector like behavior (as defined in the docs) as vectors.

The high level interface of KrylovKit is provided by the following functions:

- linsolve: solve linear systems
- eigsolve: find a few eigenvalues and corresponding eigenvectors
- geneigsolve: find a few generalized eigenvalues and corresponding vectors
- svdsolve: find a few singular values and corresponding left and right singular vectors
- exponentiate: apply the exponential of a linear map to a vector
- expintegrator : <u>exponential integrator</u> for a linear non-homogeneous ODE, computes a linear combination of the ϕ_{ij} functions which generalize $\phi_0(z) = \exp(z)$.

1 using KrylovKit

Projecting a sparse matrix into a subspace

Given $Q \in \mathbb{R}^{n imes k}$ and $Q^TQ = I$, the following statement is always true.

$$\lambda_1(Q_k^TAQ_k) \leq \lambda_1(A),$$

where $\lambda_1(A)$ is the largest eigenvalue of $A \in \mathbb{R}^{n imes n}$.

Lanczos Tridiagonalization

In the Lanczos tridiagonalizaiton process, we want to find a orthogonal matrix $oldsymbol{Q}^T$ such that

$$Q^T A Q = T$$

where $oldsymbol{T}$ is a tridiagonal matrix

$$T = egin{pmatrix} lpha_1 & eta_1 & 0 & \dots & 0 \ eta_1 & lpha_2 & eta_2 & \dots & 0 \ 0 & eta_2 & lpha_3 & \dots & 0 \ dots & dots & dots & dots & dots \ 0 & 0 & 0 & eta_{k-1} & lpha_k \end{pmatrix},$$

$$Q=[q_1|q_2|\dots|q_n],$$
 and $\operatorname{span}(\{q_1,q_2,\dots,q_k\})=\mathcal{K}(A,q_1,k).$

We have $Aq_k=eta_{k-1}q_{k-1}+lpha_kq_k+eta_kq_{k+1}$, or equivalently in the recursive style

$$q_{k+1} = (Aq_k - eta_{k-1}q_{k-1} - lpha_k q_k)/eta_k.$$

By multiplying $oldsymbol{q}_{k}^{T}$ on the left, we have

$$lpha_k = q_k^T A q_k.$$

Since q_{k+1} is normalized, we have

$$\beta_k = \|Aq_k - \beta_{k-1}q_{k-1} - \alpha_k q_k\|_2$$

If at any moment, $eta_k=0$, the interation stops due to convergence of a subspace. We have the following reducible form

$$T(eta_2=0) = egin{pmatrix} lpha_1 & eta_1 & 0 & \dots & 0 \ rac{eta_1 & lpha_2}{0} & 0 & \dots & 0 \ \hline 0 & 0 & lpha_3 & \dots & 0 \ dots & dots & dots & dots & dots \ 0 & 0 & 0 & eta_{k-1} & lpha_k \end{pmatrix},$$

A naive implementation

```
1 function lanczos(A, q1::AbstractVector{T}; abstol, maxiter) where T
        # normalize the input vector
 2
 3
        q1 = normalize(q1)
 4
        # the first iteration
 5
        q = \lceil q1 \rceil
 6
        Aq1 = A * q1
 7
        \alpha = \lceil q1' * Aq1 \rceil
        rk = Aq1 .- \alpha[1] .* q1
        \beta = \lceil norm(rk) \rceil
 9
        for k = 2:min(length(q1), maxiter)
10
             # the k-th orthonormal vector in Q
11
             push!(q, rk ./ \beta[k-1])
12
13
             Aqk = A * q[k]
             # compute the diagonal element as \alpha_k = q_k^T A q_k
14
15
             push!(\alpha, q[k]' * Aqk)
             rk = Aqk .- \alpha[k] .* q[k] .- \beta[k-1] * q[k-1]
16
             # compute the off-diagonal element as \beta_k = |r_k|
17
18
             nrk = norm(rk)
             # break if \beta_k is smaller than abstol or the maximum number of iteration is
19
             reached
             if abs(nrk) < abstol || k == length(q1)</pre>
20
21
                 break
22
             end
23
             push!(β, nrk)
24
        end
25
        # returns T and O
26
        return SymTridiagonal(\alpha, \beta), hcat(q...)
27 end
```

Example: using dominant eigensolver to study the spectral graph theory

Laplacian matrix Given a simple graph G with n vertices v_1,\ldots,v_n , its Laplacian matrix $L_{n\times n}$ is defined element-wise as

$$L_{i,j} := egin{cases} \deg(v_i) & ext{if } i = j \ -1 & ext{if } i
eq j ext{ and } v_i ext{ is adjacent to } v_j \ 0 & ext{otherwise,} \end{cases}$$

or equivalently by the matrix L=D-A, where D is the degree matrix and A is the adjacency matrix of the graph. Since G is a simple graph, A only contains 1s or 0s and its diagonal elements are all 0s.

Theorem: The number of connected components in the graph is the dimension of the nullspace of the Laplacian and the algebraic multiplicity of the o eigenvalue.

```
1 using Graphs # for generating sparse matrices
graphsize = 10
 1 graphsize = 10
One can use the Graphs.laplacian_matrix(graph) to generate a laplacian matrix (CSC formated) of
a graph.
lmat = 10×10 SparseMatrixCSC{Int64, Int64} with 40 stored entries:
                     -1
                                 -1
                                     -1
             3
                -1
                             -1
                                          -1
                 3
            -1
                    -1
                                     -1
        -1
                -1
                      3
                                              -1
                          3
                                 -1
                                         -1
                                              -1
            -1
                              3
                                 -1
                                     -1
        -1
                         -1
                                  3
                             -1
        -1
                -1
                             -1
                                      3
                                          3
            -1
                         -1
                                              -1
                     -1
                         -1
                                          -1
 1 lmat = laplacian_matrix(random_regular_graph(graphsize, 3))
  (7×7 SymTridiagonal{Float64, Vector{Float64}}:
                                                                        , 10×7 Matrix{Float64}
   2.69614 1.317
                                                                           0.322236
                                                                                       -0.1459
 1 tri, Q = lanczos(lmat, randn(graphsize); abstol=1e-8, maxiter=100)
 [4.44089e-15, 1.09679, 1.75302, 3.19394, 3.44504, 4.80194, 5.70928]
 1 eigen(tri).values
7×7 Matrix{Float64}:
  1.0
               -6.60858e-16
                              -2.66366e-16
                                                -1.66034e-15
                                                              -1.39064e-15
 -6.60858e-16
                1.0
                               5.92328e-16
                                                 8.68143e-16
                                                               2.92183e-15
                                                 1.63375e-15
 -2.66366e-16
                5.92328e-16
                               1.0
                                                              -4.23048e-15
  9.8711e-16
                5.71832e-17
                              -7.61016e-16
                                                -2.14734e-15
                                                               4.10824e-16
  1.3291e-15
               -8.89964e-16 -4.94659e-16
                                                -7.51208e-16
                                                              -3.79709e-15
                8.68143e-16
 -1.66034e-15
                               1.63375e-15
                                                 1.0
                                                               3.75926e-15
 -1.39064e-15
                2.92183e-15 -4.23048e-15
                                                 3.75926e-15
                                                               1.0
 1 Q' * Q
```

10

1 @bind graph_size Slider(10:2:200; show_value=true, default=10)

```
1 let
  2
                 graph = random_regular_graph(graph_size, 3)
  3
                 A = laplacian_matrix(graph)
                 q1 = randn(graph_size)
  5
                 tr, Q = lanczos(-A, q1; abstol=1e-8, maxiter=100)
                 # using function 'KrylovKit.eigsolve'
  6
                 @info "KrylovKit.eigsolve: " eigsolve(A, q1, 2, :SR)
  7
  8
                 @info Q' * Q
 9
                 # diagonalize the triangular matrix obtained with our naive implementation
                 @info "Naive approach: " eigen(-tr).values
11 end;
        KrylovKit.eigsolve:
        eigsolve(A, q1, 2, :SR):
                      ([3.7573e-15, 0.207694], [[-0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.0851257, -0.
        100×100 Matrix{Float64}:
            1.0
                                               2.75997e-17
                                                                                  2.43951e-16
                                                                                                                          -3.57291e-5
                                                                                                                                                                5.92405e-5
             2.75997e-17
                                               1.0
                                                                                                                             3.25787e-5
                                                                                                                                                              -0.000111796
                                                                                -1.31882e-16
             2.43951e-16
                                          -1.31882e-16
                                                                                                                          -6.16316e-5
                                                                                                                                                               9.77037e-5
                                                                                  1.0
                                                                                  1.07395e-16
          -2.33661e-16
                                               1.01501e-16
                                                                                                                             3.67231e-5
                                                                                                                                                              -0.000137275
           -1.17073e-16
                                               1.31826e-17
                                                                                  1.46956e-16
                                                                                                                          -7.80456e-5
                                                                                                                                                               0.000124429
             3.03248e-16
                                             -9.90021e-17
                                                                                -3.12135e-16
                                                                                                                             5.69881e-5
                                                                                                                                                              -0.000194713
          -1.63823e-17
                                             -2.48562e-18
                                                                               -1.49781e-16
                                                                                                                          -0.000119917
                                                                                                                                                               0.000189189
                                             -7.91477e-5
          -5.07084e-5
                                                                                -0.000114604
                                                                                                                          -1.087e-14
                                                                                                                                                              -1.74542e-15
                                                                                                                          -3.36207e-15
                                             -4.4267e-5
                                                                                -4.15905e-5
                                                                                                                                                             -1.03248e-14
          -1.69365e-5
          -1.7792e-5
                                             -5.73132e-6
                                                                                -3.55817e-5
                                                                                                                          -7.97296e-15
                                                                                                                                                             -1.1425e-15
                                                                                                                          -7.28543e-16
            1.06997e-5
                                             -3.25995e-5
                                                                                  1.55267e-5
                                                                                                                                                             -6.36023e-15
          -3.57291e-5
                                               3.25787e-5
                                                                                -6.16316e-5
                                                                                                                             1.0
                                                                                                                                                                3.11863e-16
                                                                                  9.77037e-5
             5.92405e-5
                                                                                                                             3.11863e-16
                                             -0.000111796
                                                                                                                                                                1.0
        Naive approach:
        (eigen(-tr)).values:
                      2.06155e-15, 3.95438e-10, 0.207694, 0.242399, 0.290065, 0.300134, 0.329777,
```

NOTE: with larger graph_size, you should see some "ghost" eigenvalues

Reorthogonalization

Let $r_0,\ldots,r_{k-1}\in\mathbb{R}_n$ be given and suppose that Householder matrices H_0,\ldots,H_{k-1} have been computed such that $(H_0\ldots H_{k-1})^T[r_0\mid\ldots\mid r_{k-1}]$ is upper triangular. Let $[q_1\mid\ldots\mid q_k]$ denote the first k columns of the Householderproduct $(H_0\ldots H_{k-1})$. Then $q_k^Tq_l=\delta_{kl}$ (machine precision).

The following 4 cells are copied from notebook: 5.linear-least-square.jl

```
struct HouseholderMatrix{T} <: AbstractArray{T, 2}
v::Vector{T}
β::T
end</pre>
```

```
left_mul! (generic function with 1 method)
```

```
1 # the `mul!` interfaces can take two extra factors.
2 function left_mul!(B, A::HouseholderMatrix)
3          B .-= (A.β .* A.v) * (A.v' * B)
4          return B
5 end
```

right_mul! (generic function with 1 method)

```
# the 'mul!' interfaces can take two extra factors.
function right_mul!(A, B::HouseholderMatrix)
A .= A .- (A * (B.β .* B.v)) * B.v'
return A
end
```

householder_matrix (generic function with 1 method)

```
function householder_matrix(v::AbstractVector{T}) where T

v = copy(v)

v[1] -= norm(v, 2)
return HouseholderMatrix(v, 2/norm(v, 2)^2)
end
```

The Lanczos algorithm with complete orthogonalization.

```
1 function lanczos_reorthogonalize(A, q1::AbstractVector{T}; abstol, maxiter) where T
 2
        n = length(q1)
 3
        # normalize the input vector
 4
        q1 = normalize(q1)
 5
        # the first iteration
 6
        q = [q1]
 7
        Aq1 = A * q1
        \alpha = [q1' * Aq1]
 8
        rk = Aq1 .- \alpha[1] .* q1
 9
        \beta = \lceil norm(rk) \rceil
10
        householders = [householder_matrix(q1)]
11
12
        for k = 2:min(n, maxiter)
13
            # reorthogonalize rk: 1. compute the k-th householder matrix
14
            for j = 1:k-1
15
                left_mul!(view(rk, j:n), householders[j])
16
            end
            push!(householders, householder_matrix(view(rk, k:n)))
17
18
            # reorthogonalize rk: 2. compute the k-th orthonormal vector in Q
19
            qk = zeros(T, n); qk[k] = 1 # q_k = H_1H_2...H_ke_k
            for j = k:-1:1
21
                left_mul!(view(qk, j:n), householders[j])
22
            end
23
            push!(q, qk)
24
            Aqk = A * q[k]
25
            # compute the diagonal element as \alpha_k = q_k^T A q_k
26
            push!(\alpha, q[k]' * Aqk)
            rk = Aqk .- \alpha[k] .* q[k] .- \beta[k-1] * q[k-1]
27
28
            # compute the off-diagonal element as \beta_k = |r_k|
            nrk = norm(rk)
29
30
            # break if \beta_k is smaller than abstol or the maximum number of iteration is
            reached
            if abs(nrk) < abstol || k == n</pre>
31
32
                break
33
            end
34
            push!(β, nrk)
35
        return SymTridiagonal(\alpha, \beta), hcat(q...)
36
37 end
```

```
Eigen{Float64, Float64, Matrix{Float64}, Vector{Float64}}
values:
100-element Vector{Float64}:
1.7763568394002505e-15
0.16956172619953414
0.1855972508777235
0.19833079222316918
0.20809907598807253
0.21925650648525075
0.23598987232352098
 5.765388175412039
 5.784601519769372
5.791364054663181
 5.804874546540144
5.813416104936518
5.814275574485619
vectors:
100×100 Matrix{Float64}:
 -0.0320956
              -0.0182923
                              0.0214464
                                           ... 0.0458152
                                                            0.0311769
                                                                        0.0128033
 0.0584448
               0.0314652
                             -0.0366861
                                              0.0747184
                                                            0.0510036
                                                                        0.020952
 -0.0860155
               -0.0412722
                              0.0475563
                                              0.0958827
                                                            0.0658792
                                                                        0.0270806
 0.123504
                0.0509994
                             -0.0578085
                                              0.115546
                                                            0.0801114
                                                                        0.0329607
 -0.17016
              -0.0586046
                              0.0650241
                                              0.130879
                                                            0.0918064
                                                                        0.0378161
 0.219988
               0.0604977
                             -0.0651895
                                           ... 0.144481
                                                            0.102823
                                                                        0.0424145
 -0.290813
              -0.0602284
                              0.062185
                                              0.15947
                                                            0.115522
                                                                        0.0477355
 -3.78524e-14 0.000108535
                              0.00306147
                                              0.0156465
                                                           -0.0341368
                                                                        0.0631417
                                           ... 0.0134158
 2.55036e-14 -8.54609e-5
                             -0.00245419
                                                           -0.0289428
                                                                        0.0534748
 -1.66104e-14 6.40686e-5
                              0.00186848
                                              0.0107704
                                                           -0.0230206
                                                                        0.0424936
 1.0404e-14
               -4.51643e-5
                             -0.00133359
                                              0.0082231
                                                           -0.0174512
                                                                        0.0321902
 -6.1593e-15
                2.93245e-5
                              0.000873972
                                              0.00539425
                                                           -0.0113903
                                                                        0.0209997
 2.81914e-15 -1.4215e-5
                             -0.000426037
                                              0.00271348
                                                           -0.00571204 0.0105277
 1 let
 2
       n = 1000
 3
       graph = random_regular_graph(n, 3)
       A = laplacian_matrix(graph)
       q1 = randn(n)
 5
       tr, Q = lanczos_reorthogonalize(A, q1; abstol=1e-5, maxiter=100)
 7
       @info eigsolve(A, q1, 2, :SR)
       eigen(tr)
 8
 9 end
```

Notes on Lanczos

- 1. In practise, we do not store all q vectors to save space.
- 2. Blocking technique is required if we want to compute multiple eigenvectors or a degenerate eigenvector.
- 3. Restarting technique can be used to improve the solution.

The Arnoldi Process

If A is not symmetric, then the orthogonal tridiagonalization $Q^TAQ=T$ does not exist in general. The Arnoldi approach involves the column by column generation of an orthogonal Q such that $Q^TAQ=H$ is a Hessenberg matrix.

$$H = egin{pmatrix} h_{11} & h_{12} & h_{13} & \dots & h_{1k} \ h_{21} & h_{22} & h_{23} & \dots & h_{2k} \ 0 & h_{32} & h_{33} & \dots & h_{3k} \ dots & dots & dots & \ddots & dots \ 0 & 0 & 0 & \dots & h_{kk} \end{pmatrix}$$

That is, $h_{ij}=0$ for i>j+1.

```
1 function arnoldi_iteration(A::AbstractMatrix{T}, x0::AbstractVector{T}; maxiter) where
    Τ
 2
       h = Vector{T}[]
       q = [normalize(x0)]
 3
 4
       n = length(x0)
 5
       Qassert size(A) == (n, n)
 6
       for k = 1:min(maxiter, n)
 7
           u = A * q[k]
                            # generate next vector
 8
           hk = zeros(T, k+1)
           for \mathbf{j} = 1:\mathbf{k} # subtract from new vector its components in all preceding vectors
 9
                hk[j] = q[j]' * u
10
                u = u - hk[j] * q[j]
11
12
           end
13
           hkk = norm(u)
14
           hk[k+1] = hkk
           push!(h, hk)
15
           if abs(hkk) < 1e-8 | k >=n # stop if matrix is reducible
16
17
                break
18
           else
19
                push!(q, u ./ hkk)
20
           end
21
       end
22
       # construct 'h'
23
24
       kmax = length(h)
25
       H = zeros(T, kmax, kmax)
26
       for k = 1:length(h)
27
           if k == kmax
28
                H[1:k, k] = h[k][1:k]
29
           else
30
                H[1:k+1, k] = h[k]
31
           end
32
       end
33
       return H, hcat(q...)
34 end
```

```
1 let
     n = 10
3
      A = randn(n, n)
      q1 = randn(n)
      h, q = arnoldi_iteration(A, q1; maxiter=100)
5
6
      # using function 'KrylovKit.eigsolve'
      @info "KrylovKit.eigsolve: " eigsolve(A, q1, 2, :LR)
9
      # diagonalize the triangular matrix obtained with our naive implementation
      @info "Naive approach: " eigen(h).values
11 end;
  KrylovKit.eigsolve:
  eigsolve(A, q1, 2, :LR):
       4
  Naive approach:
  (eigen(h)).values:
       -2.55741+0.0im, -1.59901+0.0im, -0.826902+0.0im, -0.586252+0.0im, 0.132536-2
```

Assignment

1. Review

I forgot to copy the definitions of rowindices, colindices and data in the following code. Can you help me figure out what are their possible values?

```
julia> sp = sparse(rowindices, colindices, data);
julia> sp.colptr
6-element Vector{Int64}:
 2
 5
 6
julia> sp.rowval
5-element Vector{Int64}:
3
 1
 1
 4
 5
julia> sp.nzval
5-element Vector{Float64}:
0.799
0.942
0.848
0.164
0.637
julia> sp.m
julia> sp.n
5
```

2. Coding (Choose one of the following two problems):

1. (easy) Implement CSC format sparse matrix-vector multiplication as function my_spv . Please include the following test code into your project.

```
using SparseArrays, Test

@testset "sparse matrix - vector multiplication" begin
    for k = 1:100
        m, n = rand(1:100, 2)
        density = rand()
        sp = sprand(m, n, density)
        v = randn(n)
        @test Matrix(sp) * v ≈ my_spv(sp, v)
    end
end
```

2. (hard) The restarting in Lanczos is a technique technique to reduce memory. Suppose we wish to calculate the largest eigenvalue of A. If $q_1 \in \mathbb{R}^n$ is a given normalized vector, then it can be refined as follows:

Step 1. Generate $q_2, \ldots, q_s \in \mathbb{R}^n$ via the block Lanczos algorithm.

Step 2. Form
$$T_s = [q_1 \mid \ldots \mid q_s]^T A[q_1 \mid \ldots \mid q_s]$$
, an s-by-s matrix.

Step 3. Compute an orthogonal matrix $U=[u_1\mid\ldots\mid u_s]$ such that $U^TT_sU=\mathrm{diag}(\theta_1,\ldots,\theta_s)$ with $\theta_1\geq\ldots\geq\theta_s$

Step 4. Set
$$q_1^{(ext{new})} = [q_1 \mid \ldots \mid q_s]u_1$$
.

Please implement a Lanczos tridiagonalization process with restarting as a Julia function. You submission should include that function as well as a test.