

Title: Lecture - Numerical Methods, PHYS 777

Speakers: Erik Schnetter, Dustin Lang

Collection/Series: Numerical Methods (Core), PHYS 777-, January 6 - February 5, 2025

Subject: Other

Date: January 09, 2025 - 10:15 AM

URL: <https://pirsa.org/25010055>

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Code Notebook Julia 1.11.2

Linear Algebra 2

- matrix types
- eigenvalues and singular values
- sparse matrices
- Krylov subspace methods
- example: the power method

[]:

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Code Notebook Julia 1.11.2

Matrix

```
[1]: A = randn(4, 4)
```

```
[1]: 4x4 Matrix{Float64}:
-0.1467  0.752702 -0.179842  0.357416
 1.03975 -0.591779  0.0324229 -1.52922
 0.539381 0.315459  0.112141  0.158221
-0.965721 -0.357836 -0.901844 -0.812315
```

```
[2]: B = (A + A') / 2
```

```
[2]: 4x4 Matrix{Float64}:
-0.1467  0.896227  0.179769 -0.304152
 0.896227 -0.591779  0.173941 -0.943526
 0.179769 0.173941  0.112141 -0.371811
-0.304152 -0.943526 -0.371811 -0.812315
```

```
[ ]: using LinearAlgebra
```

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Code Notebook Julia 1.11.2

```

0.539381  0.315459  0.112141  0.158221
-0.965721 -0.357836 -0.901844 -0.812315

[2]: B = (A + A') / 2

[2]: 4x4 Matrix{Float64}:
-0.1467  0.896227  0.179769 -0.304152
 0.896227 -0.591779  0.173941 -0.943526
 0.179769  0.173941  0.112141 -0.371811
-0.304152 -0.943526 -0.371811 -0.812315

[3]: using LinearAlgebra

[4]: Symmetric(A)

[4]: 4x4 Symmetric{Float64, Matrix{Float64}}:
-0.1467  0.752702 -0.179842  0.357416
 0.752702 -0.591779  0.0324229 -1.52922
-0.179842  0.0324229  0.112141  0.158221
 0.357416 -1.52922  0.158221 -0.812315

[5]: Diagonal(A)

[5]: 4x4 Diagonal{Float64, Vector{Float64}}:
-0.1467  .  .  .
. -0.591779  .  .

```

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Code Notebook Julia 1.11.2

```

0.752702 -0.591779 0.0324229 -1.52922
-0.179842 0.0324229 0.112141 0.158221
0.357416 -1.52922 0.158221 -0.812315

[5]: Diagonal(A)

[5]: 4×4 Diagonal{Float64, Vector{Float64}}:
-0.1467 . . .
. -0.591779 . .
. . 0.112141 .
. . . -0.812315

[7]: b = rand(4);

[8]: Diagonal(A) \ b

[8]: 4-element Vector{Float64}:
-4.322734028681198
-1.5608999672552852
4.03997938392708
-0.23387877201805332

[ ]:

```

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Code Notebook Julia 1.11.2

Eigenvalues and eigenvectors

```
[9]: eigen(A)
```

```
[9]: Eigen{ComplexF64, ComplexF64, Matrix{ComplexF64}, Vector{ComplexF64}}
values:
4-element Vector{ComplexF64}:
-1.0679978879513952 - 0.5404951051122822im
-1.0679978879513952 + 0.5404951051122822im
-0.2056048046482068 + 0.0im
 0.902947518090681 + 0.0im
vectors:
4x4 Matrix{ComplexF64}:
-0.502702+0.135156im ... -0.491863+0.0im -0.280389+0.0im
 0.760381-0.0im          0.39398+0.0im -0.722097+0.0im
-0.00801287-0.106154im  0.652982+0.0im -0.377823+0.0im
-0.105176+0.358399im   -0.420077+0.0im  0.507157+0.0im
```

```
[ ]: |
```

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Code Notebook Julia 1.11.2

```
vectors:  
4x4 Matrix{Float64}:  
-0.318948 -0.778606 0.423495 0.335704  
0.66376 -0.0440767 -0.159362 0.72944  
-0.0707617 -0.498884 -0.850378 -0.151539  
0.67282 -0.37808 0.268537 -0.576416  
[11]: eigen(Diagonal(A))  
[11]: Eigen{Float64, Float64, Matrix{Float64}, Vector{Float64}}  
values:  
4-element Vector{Float64}:  
-0.14669977917562027  
-0.5917788276417273  
0.11214059361184767  
-0.8123150492548141  
vectors:  
4x4 Matrix{Float64}:  
1.0 0.0 0.0 0.0  
0.0 1.0 0.0 0.0  
0.0 0.0 1.0 0.0  
0.0 0.0 0.0 1.0  
[ ]:
```

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Notebook Julia 1.11.2

```
[12]: SVD{Float64, Float64, Matrix{Float64}, Vector{Float64}}
U factor:
4x4 Matrix{Float64}:
-0.315989 -0.0200871 -0.846988 -0.427035
 0.903817  0.291698 -0.247296 -0.19202
-0.0476697 0.349507 -0.41367  0.839315
 0.284593 -0.890142 -0.22435  0.276262
singular values:
4-element Vector{Float64}:
 2.0732352932594
 1.6520453159998763
 0.663046853827596
 0.1171258525318271
Vt factor:
4x4 Matrix{Float64}:
 0.330667 -0.429079 -0.0848297 -0.836274
 0.819825  0.145904  0.51756  0.196802
-0.210151 -0.816535  0.452826  0.289923
 0.417593 -0.357594 -0.72103  0.421734

[ ]: C = randn(4, 3)|
```

Simple 0 3 Julia 1.11.2 | Idle Mode: Edit Ln 1, Col 16 Untitled1.ipynb 1

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Code Notebook Julia 1.11.2

```
[13]: SVD{Float64, Float64, Matrix{Float64}, Vector{Float64}}
      U factor:
      4x2 Matrix{Float64}:
      -0.0569784  0.769918
      -0.534023  0.368735
      -0.460166  -0.520824
      0.70698    0.00157886
      singular values:
      2-element Vector{Float64}:
      2.8169739017372732
      1.0154296867405945
      Vt factor:
      2x2 Matrix{Float64}:
      -0.926852  0.375428
      0.375428  0.926852

[18]: sd.V * Diagonal(sd.S) * sd.Vt

[18]: 2x2 Matrix{Float64}:
      2.56305  -0.626876
      -0.626876  1.26935
```

[]:

Simple 0 3 Julia 1.11.2 | Idle Mode: Command Ln 1, Col 1 Untitled1.ipynb 1

```
2x2 Matrix{Float64}:  
-0.926852  0.375428  
 0.375428  0.926852
```

```
[20]: sd.U * Diagonal(sd.S) * sd.Vt - C
```

```
[20]: 4x2 Matrix{Float64}:  
-5.55112e-17  1.11022e-16  
 0.0          2.77556e-17  
 0.0          0.0  
 0.0          -1.11022e-16
```

Sparse matrices

```
[ ]: |
```

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Markdown Notebook Julia 1.11.2

```
2x2 Matrix{Float64}:
-0.926852  0.375428
 0.375428  0.926852

[20]: sd.U * Diagonal(sd.S) * sd.Vt - C

[20]: 4x2 Matrix{Float64}:
-5.55112e-17  1.11022e-16
 0.0          2.77556e-17
 0.0          0.0
 0.0          -1.11022e-16
```

Sparse matrices

Storage formats:

- coordinate format (all nonzero entries and their position)
- compressed sparse column

Inefficient:

- find particular element
- add element

Simple 0 3 Julia 1.11.2 | Idle Mode: Edit Ln 8, Col 1 Untitled1.ipynb 1

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Notebook Julia 1.11.2

Sparse matrices

Storage formats:

- coordinate format (all nonzero entries and their position)
- compressed sparse column

Inefficient:

- find particular element
- add element

efficient:

- matrix-vector multiplication

```
[ ]: using SparseArrays
```

Simple 0 3 Julia 1.11.2 | Idle Mode: Edit Ln 1, Col 19 Untitled1.ipynb

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Code Notebook Julia 1.11.2

INEfficient:

- find particular element
- add element

efficient:

- matrix-vector multiplication

```
[21]: using SparseArrays
```

```
[29]: A = sprand(4, 4, 0.4)
```

```
[29]: 4x4 SparseMatrixCSC{Float64, Int64} with 7 stored entries:
 0.528813  .      .      0.0374223
 .      .      0.211107  .
 0.0010273  .      0.981117  0.597585
 .      0.843683  .      .
```

```
[23]: b = randn(4);
```

```
[24]: A * b
```

```
[24]: 4-element Vector{Float64}:
```

Simple 0 3 Julia 1.11.2 | Idle Mode: Command Ln 1, Col 14 Untitled1.ipynb 1

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Notebook Julia 1.11.2

re you have enough memory, please either convert your matrix to a dense matrix, e.g. by calling `Matrix` or if `A` can be factorized, use `\` on the dense identity matrix, e.g. `A \ Matrix{eltype(A)}(I, size(A)...)` restrictions of \ on sparse lhs applies. Alternatively, A\b is generally preferable to inv(A)*b`

Stacktrace:

```
[1] error(s::String)
  @ Base ./error.jl:35
[2] inv(A::SparseMatrixCSC{Float64, Int64})
  @ SparseArrays ~/.julia/juliaup/julia-1.11.2+0.aarch64.apple.darwin14/share/julia/stdlib/v1.11/SparseArrays/src/linalg.jl:1777
[3] top-level scope
  @ In[32]:1
```

[34]: `A \ b`

[34]: 4-element Vector{Float64}:
-0.24449743338913096
0.020911463199273925
5.686656843732336
-8.584924764127988

[]:

Simple 0 3 Julia 1.11.2 | Idle Mode: Command Ln 1, Col 1 Untitled1.ipynb 1

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Code Notebook Julia 1.11.2

```
[3] top-level scope
@ In[32]:1
```

```
[34]: A \ b
```

```
[34]: 4-element Vector{Float64}:
 -0.24449743338913096
  0.020911463199273925
  5.686656843732336
 -8.584924764127988
```

Iterative methods

```
[ ]: |
```

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Code Notebook Julia 1.11.2

```
[34]: 4-element Vector{Float64}:
      -0.24449743338913096
       0.020911463199273925
       5.686656843732336
      -8.584924764127988
```

Iterative methods

```
[ ]: # Power method
      function power_method(A)
          x = randn(size(A, 1))
          for iter in 1:20
              x = A *
          end
          return v
      end
```

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```
[34]: 4-element Vector{Float64}:
      -0.24449743338913096
       0.020911463199273925
       5.686656843732336
      -8.584924764127988
```

Iterative methods

```
[ ]: # Power method
function power_method(A)
    x = randn(size(A, 1))
    for iter in 1:20
        xnew = A * x
        eval = xnew[1] / x[1]
        err = norm(xnew - eval * x)
        x = xnew
    end
    return x
end
```

Simple 0 3 Julia 1.11.2 | Idle Mode: Edit Ln 7, Col 36 Untitled1.ipynb 1

```
[34]: 4-element Vector{Float64}:  
      -0.24449743338913096  
       0.020911463199273925  
       5.686656843732336  
      -8.584924764127988
```

Iterative methods

```
[ ]: # Power method  
function power_method(A)  
    x = randn(size(A, 1))  
    for iter in 1:20  
        xnew = A * x  
        eval = xnew[1] / x[1]  
        err = norm(xnew - eval * x)  
        println("iter: $iter  eval: $eval  error: $err")  
        x = xnew  
    end  
    return x  
end
```

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Code Notebook Julia 1.11.2

```

x = xnew
end
return x
end

```

[35]: power_method (generic function with 1 method)

[36]: power_method(Symmetric(A))

```

iter: 1  eval: 0.5376217411385715  error: 1.8128783144813911  evec: [0.6664959090425118, -1.5245795156397541,
-2.129756352606922, 0.15689137694522995]
iter: 2  eval: 0.3984988102326889  error: 2.379179312779193  evec: [0.35832269108117015, -0.4496059180382801
5, -2.3176337773117783, -1.2477685658510431]
iter: 3  eval: 0.16935426747113205  error: 3.856952123414704  evec: [0.14279116607522163, -0.489268108461939
9, -3.11443306173871, -1.371573848793906]
iter: 4  eval: -2.3430469650667956  error: 16.135704835471078  evec: [0.02418229333201792, -0.657477806875801
2, -3.9785437170571236, -1.8557948169639875]
iter: 5  eval: 2.09849114734882  error: 4.624213675315964  evec: [-0.0566602489999396, -0.8398973892827472, -
5.151210961861169, -2.3766129781298875]
iter: 6  eval: 1.4983245554670876  error: 1.527034617023125  evec: [-0.11890103093295307, -1.087455347031378
4, -6.65147813417231, -3.0804066164053725]
iter: 7  eval: 1.364690712448646  error: 0.6932471152949234  evec: [-0.17815233431719535, -1.404171857107279
7, -8.596253791961582, -3.9792729271165985]
iter: 8  eval: 1.3205427002622294  error: 0.3493400856294579  evec: [-0.2431228360437227, -1.814727103921573
8, -11.108316726763675, -5.143658955440418]
iter: 9  eval: 1.3036227429081217  error: 0.18075592090693401  evec: [-0.3210540864045889, -2.345040517749003
7, -14.255425577706212, -6.6472612600062051]

```

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```
iter: 27 eval: 1.2923249011275015 error: 1.2748764705974097e-8 evec[1]: -0.020368689526318196
iter: 28 eval: 1.2923249086464332 error: 5.228269628257325e-9 evec[1]: -0.020368689325423173
iter: 29 eval: 1.2923249117299491 error: 2.1441126900110033e-9 evec[1]: -0.020368689243036097
iter: 30 eval: 1.2923249129944985 error: 8.79300531737066e-10 evec[1]: -0.020368689209249172
iter: 31 eval: 1.29232491351309 error: 3.6060123606967693e-10 evec[1]: -0.020368689195393155
iter: 32 eval: 1.2923249137257642 error: 1.4788260107270414e-10 evec[1]: -0.0203686891897108
iter: 33 eval: 1.2923249138129822 error: 6.064648386446695e-11 evec[1]: -0.02036868918738047
iter: 34 eval: 1.29232491384875 error: 2.487111566137318e-11 evec[1]: -0.020368689186424805
iter: 35 eval: 1.2923249138634183 error: 1.0199738220863255e-11 evec[1]: -0.020368689186032882
iter: 36 eval: 1.2923249138694342 error: 4.182872503452636e-12 evec[1]: -0.020368689185872157
iter: 37 eval: 1.292324913871901 error: 1.715526367640199e-12 evec[1]: -0.020368689185806244
iter: 38 eval: 1.2923249138729125 error: 7.038089015993518e-13 evec[1]: -0.02036868918577921
iter: 39 eval: 1.2923249138733277 error: 2.886052473254436e-13 evec[1]: -0.020368689185768122
iter: 40 eval: 1.2923249138734978 error: 1.184196667743558e-13 evec[1]: -0.020368689185763577
```

[40]: 4-element Vector{Float64}:
-0.02036868918576171
-0.14660000339437243
-0.8974362345658389
-0.41557401313594233

[]:

Simple 0 \$ 3 Julia 1.11.2 | Idle Mode: Command Ln 1, Col 1 Untitled1.ipynb 1

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Code Notebook Julia 1.11.2

```
[39]: # Power method
function power_method(A)
    x = randn(size(A, 1))
    for iter in 1:40
        xnew = A * x
        eval = xnew[1] / x[1]
        err = norm(xnew - eval * x)
        println("iter: $iter eval: $eval error: $err evec[1]: $(x[1])")
        x = xnew
        x = x / norm(x)
    end
    return x
end
```

[39]: power_method (generic function with 1 method)

```
[40]: power_method(Symmetric(A))

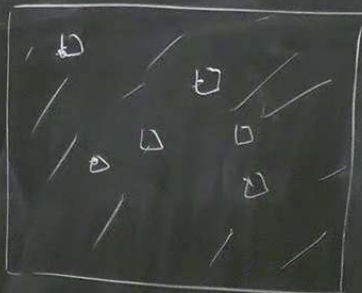
iter: 1 eval: 0.6729973992920767 error: 0.5587388394396237 evec[1]: -0.14892672035307536
iter: 2 eval: 0.49309898120705126 error: 0.6895634509682687 evec[1]: -0.5512634677517412
iter: 3 eval: 0.5824102660434007 error: 0.6642297945619118 evec[1]: -0.49249866352583704
iter: 4 eval: 0.5664484603581822 error: 0.7042162122557142 evec[1]: -0.28523494999524296
iter: 5 eval: 0.6571810481319954 error: 0.6318841513411477 evec[1]: -0.12999045077901897
iter: 6 eval: 0.7592179726058195 error: 0.5327083646511265 evec[1]: -0.06648516180827782
```

Simple 0 3 Julia 1.11.2 | Idle Mode: Command Ln 1, Col 1 Untitled1.ipynb 1

α
coectors / 1-forms

$A^{(p)}$
 $B^{(p)}$

SPARSE MATRICES



α
covectors / 1-forms

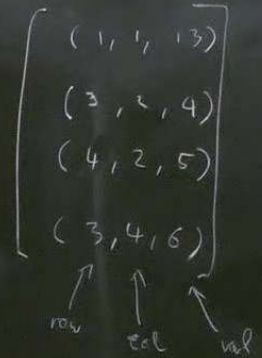
$A^{(p)}$
 $B^{(p)}$

SPARSE MATRICES



	1	2	3	4
1	13			
2				
3		4		6
4		5		

coordinate format



correctors / 1-forms

$A^{(1)}$
 $B^{(1)}$

SPARSE MATRICES

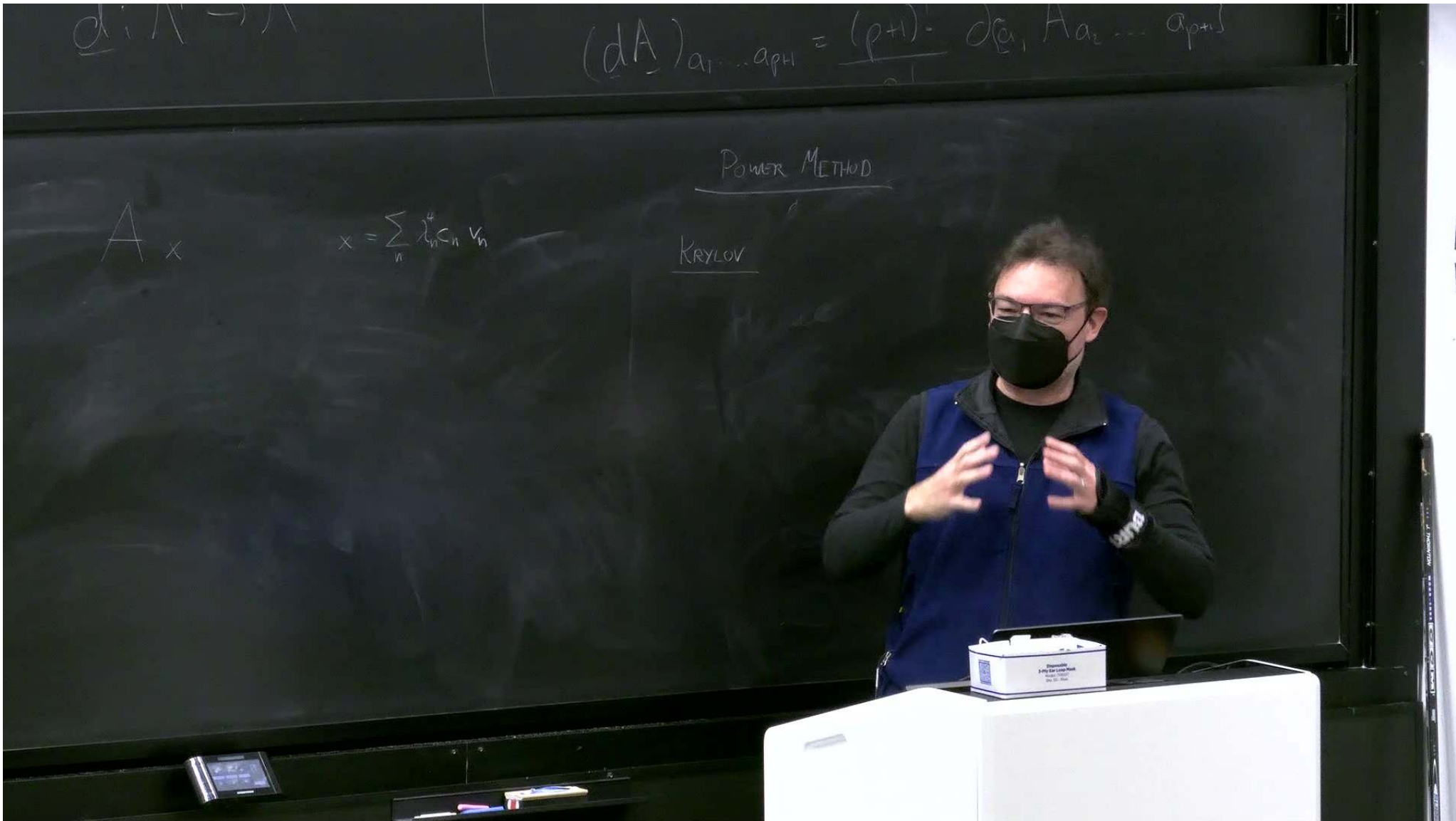
compressed sparse column (CSC)

1	2	3	4
(1,13)	(3,4)	(3,6)	
	(4,5)		

	1	2	3	4
1	13			
2				
3		4		6
4		5		

coordinate format

$\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$	$(1, 1, 13)$
	$(3, 2, 4)$
	$(4, 2, 5)$
	$(3, 4, 6)$
	row
	col
	val



Solve $Ax = b$ via iterations

Starting value x_0

$x_n \rightarrow x_{n+1}$

$$x_{n+1} = \dots A \dots x_n \dots b \dots$$

$$x_{n+1} - x_n = \alpha \cdot (A \cdot x_n - b)$$

