FYS-4096 Computational Physics, exercise 5

Return your solution to project `exercise5` under your GitLab group for this course by Friday 5 AM.

Tag the final version with `final` keyword, and make sure to include a file `problems_solved` in the repository. The `problems_solved`-file should be a comma separated list of problems you have solved.

Problems

1. Sparse matrix eigenvalues (2 XP)

Repeat problem 4 of exercise 4, but use a finer grid

```
import numpy as np
x = np.linspace(-20, 20, 2000)
```

and sparse matrices from `scipy.sparse`.

Write your code to `scripts/problem1.py`. As a starting point, you can use the example solution of `ex4 p4` available in the `material`-repository.

2. Fast matrix exponential (8 XP)

Cheapskate manager strikes again! Now we've lost our implementation of *Matrix Exponentials*. The code should calculate the operator/matrix exponential '$\exp(t\mathbf{A})\bar{\mathbf{v}}$' where '$\mathbf{A} : \mathbb{F}^N \to \mathbb{F}^N$' is a linear operator, '$\bar{\mathbf{v}} \in \mathbb{F}^N$' is a vector, and '$t \in \mathbb{F}$' is a scalar. Here the field '$\mathbb{F}$' is either the set of real numbers '$\mathbb{R}$' or complex numbers '$\mathbb{C}$'.

Help us, Brave Initiate, you're our only hope!

Implement the matrix exponential `krylov.exponential.expm_multiply` using Krylov subspace methods. The skeleton package can be found at https://www.tut.fi/fys/fys4096/expm_krylov.tar, and you can verify your implementation by passing all the unit tests (most of them are just testing the numerics so you might *occasionally* get a fail here or there).

You can get the projection matrix '$V \in \mathbb{F}^{N \times m+1}$' and the projected matrix '$H \in \mathbb{F}^{m+1 \times m}$' using the class `krylov._krylov_subspace.KrylovSubspace`, e.g.,

```
import scipy.sparse as sp
import numpy as np
from krylov._krylov_subspace import KrylovSubspace
```

```python
A = sp.rand((100,100))
v = np.random.random(100)

# Initialize the Krylov subspace
KS = KrylovSubspace(A, v)

# Do one Arnoldi iteration
KS.grow()

# Get the projection matrix and the projected operator
V, H = KS.get()
```

Note that if the Krylov subspace becomes invariant under ‘A‘, `KS.get()` will return ‘V‘ of dimensions ‘$N \times m$‘ and ‘H‘ of dimensions ‘$m \times m$‘ where ‘m‘ is the dimension of the Krylov subspace. This can also be checked with `KS.invariant` which is `False` if the subspace is not invariant and `True` when the subspace is invariant.

You can do initial testing against the following exact result:

For ‘$\mathbf{A} = \frac{1}{100}\begin{bmatrix} -50 & -49 & -48 & -47 & -46 & -45 & -44 & -43 & -42 & -41 \\ -40 & -39 & -38 & -37 & -36 & -35 & -34 & -33 & -32 & -31 \\ -30 & -29 & -28 & -27 & -26 & -25 & -24 & -23 & -22 & -21 \\ -20 & -19 & -18 & -17 & -16 & -15 & -14 & -13 & -12 & -11 \\ -10 & -9 & -8 & -7 & -6 & -5 & -4 & -3 & -2 & -1 \\ 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ 10 & 11 & 12 & 13 & 14 & 15 & 16 & 17 & 18 & 19 \\ 20 & 21 & 22 & 23 & 24 & 25 & 26 & 27 & 28 & 29 \\ 30 & 31 & 32 & 33 & 34 & 35 & 36 & 37 & 38 & 39 \\ 40 & 41 & 42 & 43 & 44 & 45 & 46 & 47 & 48 & 49 \end{bmatrix}$‘

and ‘$\overline{\mathbf{v}} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{bmatrix}$‘

we get

$$`\exp(\mathbf{A})\overline{\mathbf{v}} = \frac{1}{\sqrt[40]{e}} \begin{bmatrix} \cosh\left(\frac{\sqrt{1321}}{40}\right) - \frac{967\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ 2\cosh\left(\frac{\sqrt{1321}}{40}\right) - \frac{746\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ 3\cosh\left(\frac{\sqrt{1321}}{40}\right) - \frac{525\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ 4\cosh\left(\frac{\sqrt{1321}}{40}\right) - \frac{304\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ 5\cosh\left(\frac{\sqrt{1321}}{40}\right) - \frac{83\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ 6\cosh\left(\frac{\sqrt{1321}}{40}\right) + \frac{138\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ 7\cosh\left(\frac{\sqrt{1321}}{40}\right) + \frac{359\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ 8\cosh\left(\frac{\sqrt{1321}}{40}\right) + \frac{580\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ 9\cosh\left(\frac{\sqrt{1321}}{40}\right) + \frac{801\sinh\left(\frac{\sqrt{1321}}{40}\right)}{\sqrt{1321}} \\ \frac{2\left(6605\cosh\left(\frac{\sqrt{1321}}{40}\right)+511\sqrt{1321}\sinh\left(\frac{\sqrt{1321}}{40}\right)\right)}{1321} \end{bmatrix} \approx \begin{bmatrix} -25.55275755133941 \\ -17.98505499928794 \\ -10.41735244723646 \\ -2.849649895184989 \\ 4.718052656866485 \\ 12.28575520891796 \\ 19.85345776096943 \\ 27.42116031302091 \\ 34.98886286507238 \\ 42.55656541712385 \end{bmatrix}`$$