MATH 5344 - PROGRAMMING PROBLEM 3

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1. System Information

System: Nick Moore's Desktop "NickArch"			
Software			
OS	**Python version**	**Numpy version**	**SciPy version**
Arch Linux (Kernel 5.9.9)	3.8.6	1.19.4	1.5.4
Processor Information			
Processor		**Number of Cores**	**Speed**
AMD Ryzen 7 3800X		8 (16 Threads)	3.9GHz Base, Boost to 4.5GHz
Memory Information			
Main RAM		**L2**	**L3**
32 GB @ 3000MHz DDR4		512KB per core	32MB

2. Results from DH CG

Almost all runs of PCG with a drop tolerance or 1 and 0.1 did not converge, even after 1000000 iterations, so those results are omitted. The maximum CG iterations allowed for the following results was 10000.

Matrix: Debye-Huckel #9									
Size: 289×289									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	11	2.72e-07	5.65e-06	0.000807	0.000713	0.00152	3.62e-16	1.38e-14	0.000812
0.001	3	4.10e-07	6.11e-06	0.000862	0.000247	0.00111	3.62e-16	1.38e-14	0.000812
0.0001	2	4.36e-07	2.77e-06	0.000829	0.000188	0.00102	3.62e-16	1.38e-14	0.000812
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	15	3.38e-09	1.42e-08	0.000825	0.00087	0.0017	3.62e-16	1.38e-14	0.000812
0.001	4	5.81e-09	3.75e-08	0.00082	0.000306	0.00113	3.62e-16	1.38e-14	0.000812
0.0001	3	1.83e-10	5.79e-09	0.000815	0.000244	0.00106	3.62e-16	1.38e-14	0.000812

Matrix: Debye-Huckel #10									
Size: 545×545									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	12	5.94e-07	2.77e-05	0.00163	0.00151	0.00314	3.46e-16	2.95e-14	0.00151
0.001	4	1.58e-07	4.11e-06	0.00167	0.00064	0.00231	3.46e-16	2.95e-14	0.00151
0.0001	2	3.46e-07	1.28e-06	0.00165	0.000384	0.00204	3.46e-16	2.95e-14	0.00151
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	18	7.29e-09	5.08e-07	0.00164	0.0022	0.00384	3.46e-16	2.95e-14	0.00151
0.001	5	2.62e-09	9.71e-09	0.00123	0.00049	0.00172	3.46e-16	2.95e-14	0.00151
0.0001	3	5.21e-11	2.52e-09	0.00121	0.000341	0.00155	3.46e-16	2.95e-14	0.00151

Matrix: Debye-Huckel #11									
Size: 1089×1089									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	24	5.62e-07	1.34e-04	0.00259	0.00246	0.00505	3.64e-16	8.78e-15	0.00244
0.001	6	7.22e-08	1.86e-05	0.0028	0.000788	0.00359	3.64e-16	8.78e-15	0.00244
0.0001	2	2.14e-07	2.90e-06	0.0028	0.000364	0.00317	3.64e-16	8.78e-15	0.00244
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	40	3.70e-09	7.75e-07	0.00263	0.00395	0.00659	3.64e-16	8.78e-15	0.00244
0.001	9	4.37e-09	4.25e-07	0.00277	0.0011	0.00387	3.64e-16	8.78e-15	0.00244
0.0001	3	1.74e-10	4.04e-09	0.00277	0.000466	0.00324	3.64e-16	8.78e-15	0.00244

Matrix: Debye-Huckel #12									
Size: 2113×2113									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	23	4.87e-07	7.60e-05	0.00585	0.00484	0.0107	3.89e-16	2.31e-14	0.00559
0.001	7	4.39e-07	5.61e-05	0.0066	0.00186	0.00846	3.89e-16	2.31e-14	0.00559
0.0001	3	3.07e-08	3.32e-06	0.00674	0.000998	0.00774	3.89e-16	2.31e-14	0.00559
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	35	4.87e-09	1.02e-06	0.00588	0.00716	0.013	3.89e-16	2.31e-14	0.00559
0.001	11	1.67e-09	9.14e-07	0.00653	0.00275	0.00928	3.89e-16	2.31e-14	0.00559
0.0001	4	2.46e-09	9.65e-08	0.00675	0.00124	0.00799	3.89e-16	2.31e-14	0.00559

Matrix: Debye-Huckel #13									
Size: 4225×4225									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	32	9.08e-07	3.52e-05	0.0123	0.0117	0.024	4.24e-16	1.01e-13	0.0122
0.001	10	1.85e-07	4.40e-06	0.0145	0.00452	0.019	4.24e-16	1.01e-13	0.0122
0.0001	3	4.91e-07	2.60e-05	0.0153	0.0018	0.0171	4.24e-16	1.01e-13	0.0122
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	52	7.57e-09	1.60e-07	0.0125	0.0187	0.0312	4.24e-16	1.01e-13	0.0122
0.001	12	9.36e-09	2.70e-06	0.0144	0.00534	0.0197	4.24e-16	1.01e-13	0.0122
0.0001	5	5.33e-09	1.68e-07	0.0153	0.00267	0.018	4.24e-16	1.01e-13	0.0122

Matrix: Debye-Huckel #14									
Size: 8321×8321									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	31	5.81e-07	6.90e-04	0.039	0.0328	0.0717	4.44e-16	1.43e-13	0.0361
0.001	13	7.92e-07	2.47e-05	0.0358	0.0121	0.0479	4.44e-16	1.43e-13	0.0361
0.0001	4	2.79e-07	3.19e-04	0.0403	0.00487	0.0452	4.44e-16	1.43e-13	0.0361
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	59	5.32e-09	1.26e-06	0.0281	0.0433	0.0715	4.44e-16	1.43e-13	0.0361
0.001	21	1.80e-09	1.82e-07	0.035	0.0183	0.0532	4.44e-16	1.43e-13	0.0361
0.0001	6	5.56e-09	4.82e-07	0.0395	0.00681	0.0463	4.44e-16	1.43e-13	0.0361

Matrix: Debye-Huckel #15									
Size: 16641×16641									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	44	7.06e-07	1.23e-03	0.0825	0.0769	0.159	4.77e-16	9.31e-14	0.105
0.001	13	5.73e-07	1.55e-03	0.0802	0.0292	0.109	4.77e-16	9.31e-14	0.105
0.0001	7	8.82e-08	1.77e-05	0.0961	0.0213	0.117	4.77e-16	9.31e-14	0.105
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	84	8.36e-09	7.80e-06	0.0641	0.146	0.21	4.77e-16	9.31e-14	0.105
0.001	22	4.80e-09	4.07e-06	0.0802	0.0471	0.127	4.77e-16	9.31e-14	0.105
0.0001	8	9.20e-09	1.32e-05	0.0957	0.0271	0.123	4.77e-16	9.31e-14	0.105

Matrix: Debye-Huckel #16									
Size: 65137×65137									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	82	9.89e-07	1.37e-03	0.295	0.561	0.855	5.40e-16	6.52e-13	0.808
0.001	23	8.00e-07	1.10e-03	0.385	0.248	0.633	5.40e-16	6.52e-13	0.808
0.0001	11	2.32e-07	8.00e-05	0.514	0.171	0.685	5.40e-16	6.52e-13	0.808
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	257	9.79e-09	1.24e-05	0.283	1.75	2.03	5.40e-16	6.52e-13	0.808
0.001	39	5.42e-09	3.20e-06	0.38	0.423	0.802	5.40e-16	6.52e-13	0.808
0.0001	14	6.78e-09	1.01e-05	0.503	0.208	0.711	5.40e-16	6.52e-13	0.808

Matrix: Debye-Huckel #17									
Size: 95538×95538									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	109	9.99e-07	9.32e-04	0.497	1.2	1.7	5.23e-16	5.62e-13	1.39
0.001	26	8.79e-07	4.20e-04	0.643	0.416	1.06	5.23e-16	5.62e-13	1.39
0.0001	13	4.27e-07	2.00e-04	0.85	0.277	1.13	5.23e-16	5.62e-13	1.39
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	498	9.89e-09	1.44e-05	0.49	5.47	5.96	5.23e-16	5.62e-13	1.39
0.001	47	8.99e-09	1.61e-06	0.641	0.745	1.39	5.23e-16	5.62e-13	1.39
0.0001	21	7.25e-09	2.21e-06	0.848	0.462	1.31	5.23e-16	5.62e-13	1.39

Matrix: Debye-Huckel #18									
Size: 197830×197830									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	140	9.93e-07	1.34e-03	1.21	3.22	4.43	6.15e-16	2.09e-12	5.2
0.001	41	9.30e-07	3.11e-04	1.66	1.47	3.13	6.15e-16	2.09e-12	5.2
0.0001	14	5.58e-07	4.47e-03	2.52	0.719	3.24	6.15e-16	2.09e-12	5.2
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	10000	2.51e-08	1.35e-05	1.21	227	228	6.15e-16	2.09e-12	5.2
0.001	52	8.52e-09	5.74e-05	1.64	1.84	3.48	6.15e-16	2.09e-12	5.2
0.0001	25	9.67e-09	5.25e-05	2.49	1.22	3.71	6.15e-16	2.09e-12	5.2

Matrix: Debye-Huckel #19									
Size: 436218×436218									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	252	9.89e-07	1.41e-03	2.83	13	15.8	5.63e-16	5.46e-12	12.8
0.001	44	8.86e-07	1.19e-03	4.21	3.34	7.55	5.63e-16	5.46e-12	12.8
0.0001	18	5.56e-07	1.69e-03	7.09	1.87	8.96	5.63e-16	5.46e-12	12.8
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	10000	4.18e-07	4.03e-05	2.81	514	517	5.63e-16	5.46e-12	12.8
0.001	94	9.32e-09	3.07e-06	4.21	7.03	11.2	5.63e-16	5.46e-12	12.8
0.0001	32	7.14e-09	4.73e-06	7.07	3.25	10.3	5.63e-16	5.46e-12	12.8

Matrix: Debye-Huckel #20									
Size: 769494×769494									
Solver: PCG									
Preconditioning: ILU right, `fill_factor=30`									
Stopping tolerance: $\tau = 10^{-6}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	411	9.96e-07	1.34e-03	6.22	39.3	45.5	6.46e-16	2.11e-11	42.6
0.001	56	8.35e-07	1.65e-03	10.8	7.96	18.7	6.46e-16	2.11e-11	42.6
0.0001	21	6.68e-07	2.21e-03	17.7	4.1	21.8	6.46e-16	2.11e-11	42.6
Stopping tolerance: $\tau = 10^{-8}$									
	Convergence			Iterative solve time			Direct solve		
Fill drop tol.	Iters	$\|r_{\text{final}}\|$	$\|e\|$	Build ILU	PCG	total	$\|r\|$	$\|e\|$	time
0.01	10000	5.44e-07	6.05e-04	6.23	956	962	6.46e-16	2.11e-11	42.6
0.001	99	9.16e-09	1.92e-04	10.7	13.9	24.6	6.46e-16	2.11e-11	42.6
0.0001	39	9.68e-09	1.47e-05	17.6	7.37	25	6.46e-16	2.11e-11	42.6

3. Analysis

Preconditioned CG with the correct drop tolerance appears to always achieve the desired accuracy in a quicker time than the Direct Solve. It does depend on the drop tolerance. It should also be noted that at the larger drop tolerances, 0.1 and 1, the CG method did not converge, even with a large number of maximum iterations. Also, we larger matrices, the performance of the 0.01 drop tolerance also started to suffer. In a couple of cases, the number of iterations required exceeded 10000, leading to large timings. The smaller drop tolerances however were very effective, often twice as fast as the direct method, even for the larger matrices.

Even in larger sizes, the direct solver is still able to achieve a residual of around machine epsilon. Even at high fill drop tolerance, the preconditioner performance is still improving, so there does not appear to be any roundoff issues.

4. Error Analysis

The original problem called for calculating the condition number using `np.linalg.cond`, but this function requires a dense matrix, severely limiting the capability to calculate the condition number of the larger matrices. Even on my machine with 32G of ram, matrix 16 was too large to fit.

As an alternative, we can use a spare function to approximate the largest and smallest eigenvalues of a sparse matrix. The code is given below:

```
import scipy.sparse.linalg as splu
evl, _ = splu.eigs(A, which='LM')
evs, _ = splu.eigs(A, sigma=1e-8)
evl = abs(evl)
evs = abs(evs)
condNum = evl.max()/evs.min()
```

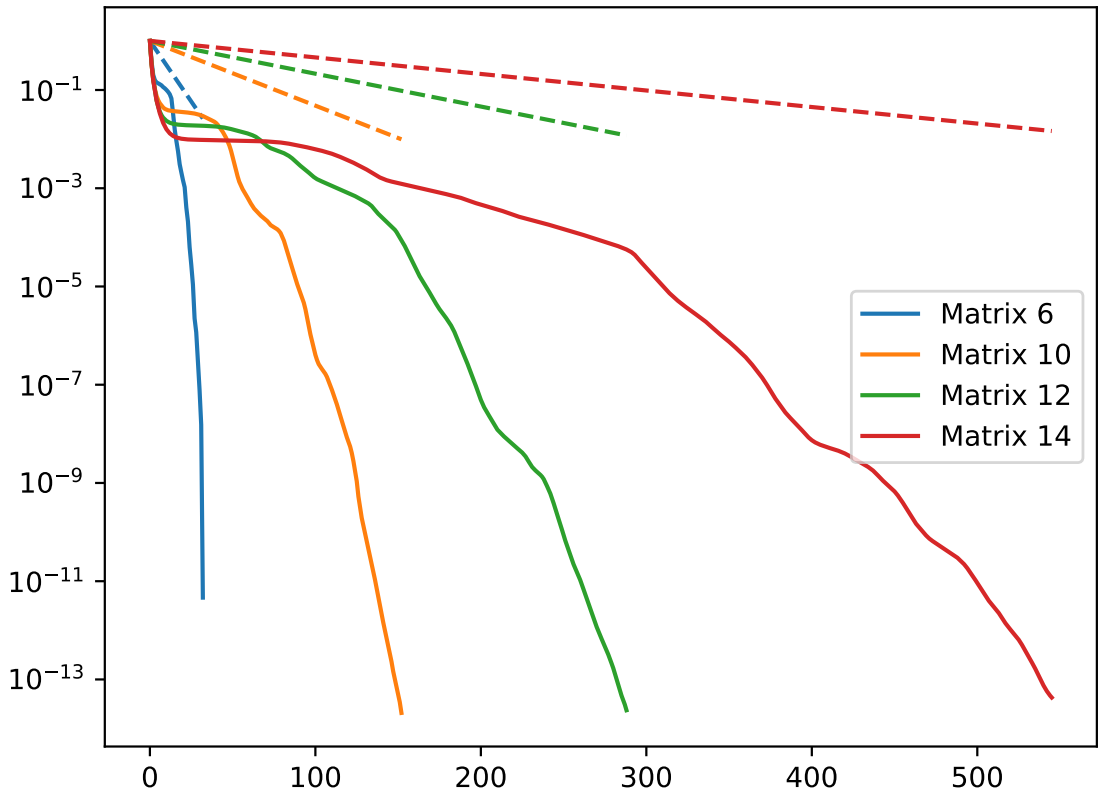
The `eigs` function uses the Implicitly Restarted Arnoldi Method to find eigenvalues and eigenvectors. The `evl` finds the "Largest Magnitude (LM)" eigenvalue, while the `evs` finds the eigenvalue

closest to `sigma = 1e-8` using a shift-invert mode. See the documentation at this link for more information.

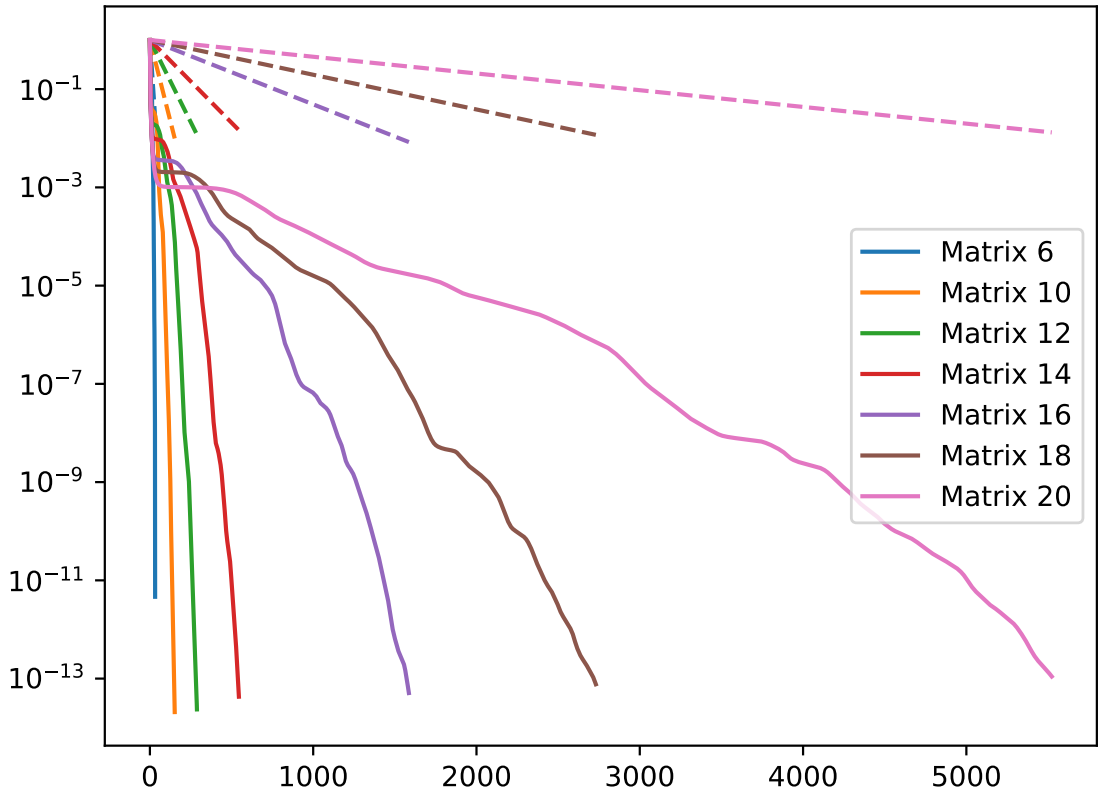
I tested this value against the value calculated from `np.linalg.cond` for matrices 6, 10, 12, and 14. The results were all within `1e-1` and calculated significantly faster as well. Below I have included the condition numbers for selected matrices as well as the timing information using the above code:

Matrix	κ	time (sec)
6	309.9087	0.004374
10	4341.4415	0.03849
12	16885.3977	0.1048
14	66549.3821	0.4535
16	439719.3065	8.8969
18	1509783.0976	12.7406
20	6507442.3003	81.0556

Using these conditions number and adapting the PCG code to calculate the relative A-norm of the error, we can plot these errors as a function of iteration count. First, the four required in the original problem statement. In the figure below, the solid lines are the calculated relative error and the dashed lines are the theoretical error bound:



Next, since the condition numbers for the larger matrices were also determined, we can plot the results for the larger matrices as well:



In all cases, we do see that the error never exceeds the theoretical bound and especially for the larger matrices, tends to be much lower.