Homework 2

1. Create problems and solutions on the course training wiki:

   - In Block 2-3: x exercise problems (per person), without solutions
   - In Block 2-3: x solutions (per person) to problems which do not yet have a solution. Don't do the problems you created.

   If you are attending SF2524 $x = 2$. If you are attending SF3580 $x = 3$. If you are attending SF3580 and have completed SF2524 in your master studies, $x = 4$.

SF2524: If you do not want bonus points, you may skip exercise 1

2. Implement GMRES (Generalized Minumum Residual method) based on the Arnoldi method, with good orthogonalization, that you developed in Homework 1. Consider the linear system $Ax = b$, where A and b are generated by

```
alpha=5;  m=100; rand('state',5);
A = sprand(m,m,0.5);
A = A + alpha*speye(m); A=A/norm(A,1);
b = rand(m,1);
```

(a) Plot the norm of the error as a function of iteration as well as the residual norm (with `semilogy`). You may in this exercise use `A\b` as an exact solution. Generate figures for the values $\alpha = 1, 5, 10, 100$.

(b) Plot the eigenvalues with `plot(eig(full(A)),'*')` for all choices of α in (a) and provide provide a bound for the convergence factor. Relate the observed convergence to the convergence theory by plotting the estimated convergence factor (predicted by the eigenvalues) in convergence figures as in (a).

(c) Generate the following table, where `resnorm`$=\|Ax - b\|_2$ and `time` is the CPU-time and n is the number of iterations. Make the corresponding simulations for the backslash operator `\`. Make tables for $\alpha = 1$ and $\alpha = 100$. (You may want to extend table, if your computer allows it.)

The matlab backslash-command is based on extremely optimized LU-factorizations (or sometimes Cholesky factorizations or Cholesky decompositions).

GMRES

	$m=100$		$m=200$		$m=500$	
	resnorm	time	resnorm	time	resnorm	time
$n=5$						
$n=10$						
$n=20$						
$n=50$						
$n=100$						

Backslash

	$m=100$		$m=200$		$m=500$	
	resnorm	time	resnorm	time	resnorm	time

(d) Suppose we are in a situation where it is sufficient to compute a solution to accuracy (relative residual norm) 10^{-5}. Is GMRES better than the backslash operator in this situation? Depending on your specific computer, you may want to extend/modify the table in c) to support your claim.

3. Do canvas quiz "Quiz Homework 2" `https://kth.instructure.com/courses/6945/quizzes`. This task should be done individually.

4. In this exercise you shall computationally verify the theoretical orthogonality and minimization properties of CG and GMRES. Consider the linear system of equations

$$\begin{bmatrix} 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 \end{bmatrix} x = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

(a) Compute α, β, γ such that $\operatorname{span}(x_1, x_2, x_3, x_4) = \operatorname{span}(c_0, c_1, c_2, c_3)$ where $c_0, \ldots, c_3$ have the structure

$$C = [c_0, c_1, c_2, c_3] = \begin{bmatrix} 1 & \alpha & 0 & \gamma \\ 1 & 0 & \beta & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 7 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

and $x_0, \ldots, x_3$ are the iterates of the conjugate gradient method for this linear system. This can be solved without a computer.

Hint: Consider the Krylov matrix K_n and use theory about the span of the iterates in the conjugate gradient method.

(b) Implement CG for this problem (TB Algorithm 38.1) and verify the minimization property as follows. In the following code, replace `???` with appropriate formulas such that `x_fmin` and `x_cg` become equal (at least in exact arithmetic and if fminsearch solves the problem exactly).

```
alpha=??; beta=??; gamma=??;
C=[1 alpha 0    gamma
   1 0     beta 0
   0 1     0    0
   0 0     1    7
   0 0     0    1
   0 0     0    0
   0 0     0    0
   0 0     0    0];
opts = optimset('TolFun',1e-10);
z=fminsearch(@(z) ??? ,  [1;1;1;1],opts);
x_fmin=C*z;
x_cg=cg(A,b,m);
```

Select `m` such that `x_cg` is an element of the Krylov subspace of dimension four.

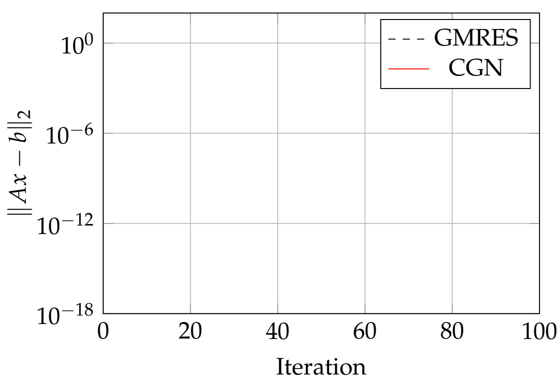
(c) Make the same experiment as in (b) for GMRES, by changing `???` in `z=fminsearch(@(z) ??? ,  [1;1;1;1],opts)` such that `C*z` becomes the approximation generated by GMRES.

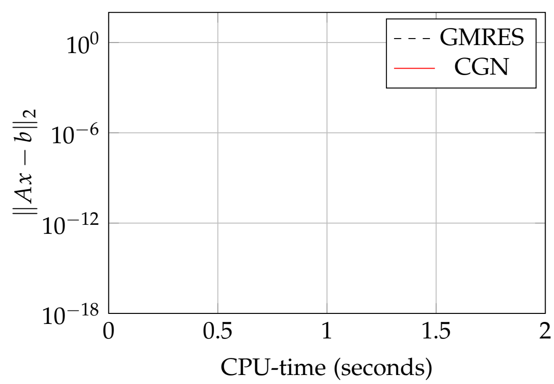
If you are doing the homeworks in the Julia programming language, you can use the package Optim instead of fminsearch. See page "Julia instructions" on CANVAS.

5. Suppose A is a real symmetric matrix with eigenvalues $10, 10.5$ and 100 eigenvalues in the interval $[2, 3]$. Prove a bound on how many steps of CG must be carried out in order to reduce the error (measured in $\|Ax_n - b\|_{A^{-1}} = \|x_n - x_*\|_A$) by a factor 10^7. You may assume exact arithmetic and that no premature breakdown occurs.

6. In following problem we use the the matrices `B` and `b` given in the mat-file: `http://www.math.kth.se/na/SF2524/matber15/Bwedge2.mat`

   (a) Compare GMRES and CGN for this problem by completing following two figures. Note that both figures illustrate the same simulation, but with different x-axis. The second figure highly depends on the computing environment, so it may be necessary to adjust the limits of the x-axis.





   (b) Relate the result in (a) to the convergence theory for CGN and GMRES?

Only for PhD students taking the course *Numerical linear algebra*:

7. In the lectures we derived convergence bounds of GMRES for diagonalizable matrices. In this exercise you shall show convergence for a class of non-diagonalizable matrices. Suppose $A \in \mathbb{C}^{m\times m}$ is invertible and suppose $\lambda_1 = \lambda_2$ is a double eigenvalue and all other eigenvalues are distinct. Assume that λ_1 has a Jordan block of size two. Moreover, suppose all eigenvalues λ_i, $i = 1, \ldots, m$ are contained in an open disk of radius $\rho > 0$ centered at $c \in \mathbb{C}$, such that $\lambda_i \in C(\rho, c)$ for all $i = 1, \ldots, m$. Assume $|\rho| < |c|$ and $\lambda_1 \neq c$.

Recall from the definition of the Jordan canonical form: If the eigenvalue λ_1 has one Jordan block of size two and all other Jordan blocks are of size one we have the following factorization. There exists an invertible matrix $V \in \mathbb{C}^{m\times m}$ and a matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & 1 & & & \\ & \lambda_1 & 0 & & \\ & & \lambda_3 & \ddots & \\ & & & \ddots & 0 \\ & & & & \lambda_m \end{pmatrix}.$$

such that $A = V\Lambda V^{-1}$.

   (a) Let $V\Lambda V^{-1} = A$ be the Jordan canonical form. Prove

$$\min_{p\in P_n^0} \|p(A)\| \leq \|V\|\|V^{-1}\| \min_{p\in P_n^0} \|p(\Lambda)\|$$

   (b) Prove that for any polynomial $p(z) = a_0 + a_1 z + \cdots + a_n z^n$,

$$p\left(\begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix}\right) = \begin{pmatrix} p(\lambda_1) & p'(\lambda_1) \\ 0 & p(\lambda_1) \end{pmatrix}.$$

   (c) Prove

$$\|p(\Lambda)\| = \max\left(\left\|\begin{pmatrix} p(\lambda_1) & p'(\lambda_1) \\ 0 & p(\lambda_1) \end{pmatrix}\right\|, |p(\lambda_3)|, |p(\lambda_4)|, \ldots, |p(\lambda_m)|\right)$$

Hint for (c): Show that the 2-norm of a block diagonal matrix is the maximum of the two-norm of the blocks by using the formula for the two-norm in terms of singular values.

(d) Determine α_n and β_n such that

$$p(z) = (\alpha_n + \beta_n z)\frac{(c-z)^{n-1}}{c^{n-1}}$$

satisfies $p \in P_n^0$ and $p'(\lambda_1) = 0$ for all $n > 1$.

(e) Combine (a)-(d) and determine a *bounded* sequence $[\gamma_n]_{n=1}^{\infty}$ such that

$$\frac{\|Ax_n - b\|}{\|b\|} \leq \|V\|\|V^{-1}\|\gamma_n \frac{\rho^n}{|c|^n}$$

for all $n > 0$.

(f) Is there a penalty to have double eigenvalues in the sense of bounds, i.e., is the asymptotic convergence predicted in (e) faster than the prediction we derived for diagonalizable matrices? In particular, what happens when we carry out many iterations, i.e., when $n \to \infty$?

(e) Show the above (a)-(f) to a PhD colleague. Check each others reasoning for clarity in preciseness. In the hand-in, specify who you have showed it to.

From lectures: $P_n^0 = \{p \in P_n : p(0) = 1\}$ where P_n is the set of polynomials of degree less or equal to n.

Connection with current research: Researchers in numerical linear algebra are actively working on gaining further understanding of $\|p(A)\|$. The set $W(A) = \{\frac{x^*Ax}{x^*x} : x \in \mathbb{C}^m\}$ is called the field of values of A. It has been shown that $\|p(A)\| \leq \alpha \cdot \max_{z \in W(A)} |p(z)|$ holds for $\alpha = 11.08$. The open problem called Crouzeix's conjecture states that the bound holds for $\alpha = 2$. What happens if A is a Jordan block of size two with $\lambda_1 = \lambda_2 = 0$ and $p(z) = z$? Can you show that α cannot be smaller than 2? *Spoiler alert* See presentation at an important conference: `http://sites.uclouvain.be/HHXIX/Plenaries/Overton.pdf`

8. Only for PhD students attending SF3580 and have attended SF2524 in their Master studies: GMRES can be adapted to incorporate a starting value (called x_0), which should be selected as a vector approximating the solution to $Ax = b$. We try to find a correction which is an element of a Krylov subspace such that we instead define the approximations as

$$\min_{x \in \mathcal{K}(A,f)+x_0} \|Ax - b\|_2 = \|Ax_n - b\|_2,$$

which reduces to the definition of GMRES-iterates if we select $x_0 = 0$ and $f = b$.

(a) Suppose $AQ_n = Q_{n+1}\underline{H}_n$ is an Arnoldi factorization. How should f be selected such that we can generalize lemma in lecture notes and

$$x_n = Q_n z + f$$

(b) Suppose A is diagonalizable and generalize the min-max bound

(c) Use the above as a procedure to carry out explicit restarting and illustrate it with an example.