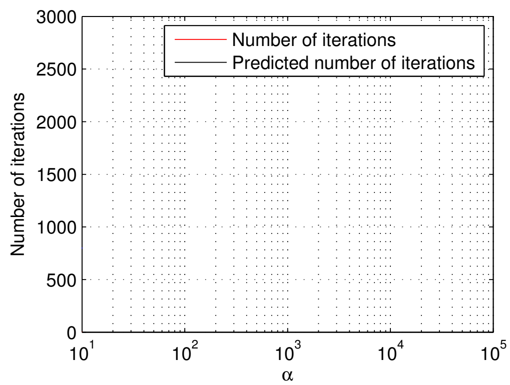
Homework 3

Deadline (for bonus points): 2015-12-10

1. **Exercise about basic QR-method.** Implement the basic QR-method. Apply it to `alpha_example.m` from the course web page. Measure the error with the maximum value below the diagonal `errfun=@(A) max(max(abs(tril(A,-1))))`.

   (a) Plot the number of iterations required to achieve error 10^{-10}, as a function of α. More precisely, generate the following plot.



For the theoretical reasoning in (b) and (c) you may use the function `eig`

   (b) Suppose the eigenvalues are ordered by magnitude $|\lambda_1| < \cdots < |\lambda_m|$. From the lecture notes we know that the elements below the diagonal will asymptotically after n iterations be proportional to $|\lambda_i/\lambda_j|^n$ with $i < j$. For large α the error will be dominated by one particular choice of i and j. Which ones?

   (c) Use (b) to establish an estimated number of iterations required to reach a specified tolerance, for different choices of α. Add a plot of the predicted number of iterations in the plot generated in (a), for tolerance 10^{-10}, and discuss the result.

Hint for (c): Show that if the error behaves as $e_k = |\beta|^k$, then $e_N = \mathtt{TOL}$ if $N = \ln(\mathtt{TOL})/\ln(|\beta|)$.

2. **Exercises about Hessenberg reduction and shifted QR-method.**

Hint for (a): First derive a formula first for the case $\|y\| = 1$.

   (a) Generalize Lemma 2.2.3 in the lecture notes as follows. Given a vector $x \in \mathbb{R}^n$ and a vector $y \in \mathbb{R}^n$ with $y \neq 0$ and $x \neq 0$, derive a formula for a Householder reflector (represented by a normal direction $u \in \mathbb{R}^n$) such that $Px = \alpha y$ for some value α.

(b) Implement a naive (inefficient) Hessenberg reduction by completing the program `naive_hessenberg_red.m` on the course web page.

(c) Implement Algorithm 2 in the lecture notes and compare the computation time with the algorithm in (b). Carry out the comparison by computing a Hessenberg reduction of `A=alpha_example(1,m)`, which generates an $m \times m$-matrix. Complete the following table.

	CPU-time Algorithm 2	CPU-time of algorithm in (b)
m=10		
m=100		
m=200		
m=300		
m=400		

(d) Let $\bar{H}$ be the result of one step of the shifted QR-method with shift σ for the matrix

$$A = \begin{bmatrix} 3 & 2 \\ \varepsilon & 1 \end{bmatrix}.$$

Run the shifted QR for two different choices of σ and complete the following table

ε	$\lvert\bar{h}_{2,1}\rvert$	
	$\sigma = 0$	$\sigma = a_{2,2}$
0.4	0.0961	0.0769
0.1		
0.01		
$\vdots$		
10^{-10}		
0		

Interpret the result in the table. What do the values in the table correspond to? Which choice of σ is better in this case?

Hint: What does the shifted QR-method reduce to when you select $\sigma = 0$?

3. Download the template `schur_parlett.m` from the course web page

(a) Complete the template code and compute $\sin(A)$ where

$$A = \begin{bmatrix} 1 & 4 & 4 \\ 3 & -1 & 3 \\ -1 & 4 & 4 \end{bmatrix}$$

(b) Let `A=rand(100,100)`. Use the Schur-Parlett method from (a) to compute A^N, and compare with the naive method to compute A^N:

```
B=A; for i=1:N-1; B=B*A; end.
```

Complete the following table. Increase N until you see that the best method changes, or see a tendency.

	CPU-time naive	CPU-time Schur-Parlett
N=2		
N=10		
N=100		
N=200		
$\vdots$		

The MATLAB command `A^N` for large N will actually not do the naive method but do a procedure similar to Schur-Parlett.

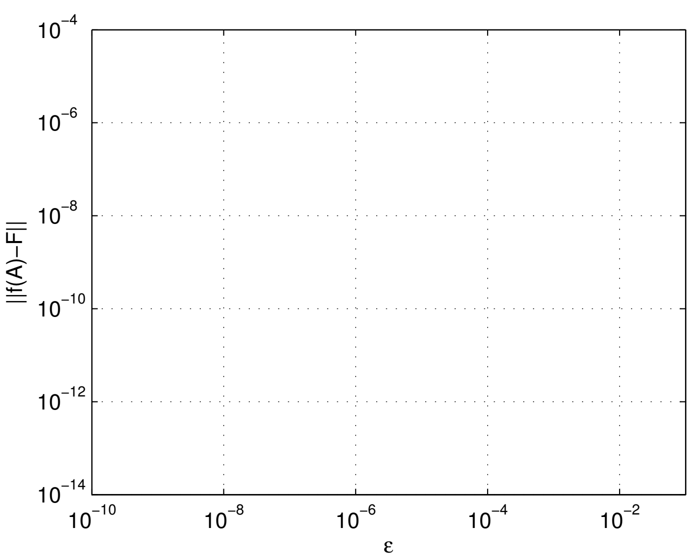
(c) What are the computational complexities of the two methods in (b) as a function of the size of the matrix and N?

4. Let $A = \begin{bmatrix} \pi & 1 \\ 0 & \pi+\varepsilon \end{bmatrix}$ where $\varepsilon > 0$.

(a) Prove (for instance using the Jordan definition) that if p is a polynomial which interpolates g in the eigenvalues of A, then $p(A) = g(A)$. Find exact expressions for α and β when $p(z) = \alpha + \beta z$ for the matrix A.

(b) Give a formula for the exact value of $\exp(A)$ using (a).

(c) Let F be the result of computing $\exp(A)$ with the Jordan definition as in the last example in Section 3.1.2. Compare the exact result in (b) with the computed value for different ε. Generate the following figure (using `loglog()`) and explain the result.



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

5. **Exercise about exploitation of structure in specific application.** The purpose of this exercise is to learn some techniques to derive more efficient methods by taking problem-specific structure into account. (The new method you will derive is not necessarily in general the best for this problem-type.)

   (a) Prove that

   $$\frac{d}{dt}\exp(tA) = A\exp(tA) = \exp(tA)A$$

   (b) Let $G(t) := \exp(-tA)B\exp(tA)$ and let $[\cdot,\cdot]$ denote a commutator, i.e., $[A,B] := AB - BA$. Show that

   $$G(t) = B + t[B,A] + \frac{t^2}{2!}[[B,A],A] + \frac{t^3}{3!}[[[B,A],A],A] + \cdots \quad (*)$$

   (c) Suppose A is anti-symmetric $A^T = -A$. Let

   $$P := \int_0^\tau \exp(tA^T)B\exp(tA)\,dt$$

   Derive an expression for P involving commutators of A and B.

   (d) Let $C_k = [C_{k-1}, A]$ with $C_0 = B$. Show that $\|C_k\| \le 2^k\|A\|^k\|B\|$.

   (e) Suppose $\|A\| < \frac{1}{2}$ and $t \le 1$. Let G_N be the truncation of G,

   $$G_N(t) := B + t[B,A] + \cdots + \frac{t^N}{N!}[\cdots[[B,A],A]\cdots,A].$$

   Derive a bound for $\|G_N(t) - G(t)\|$, which converges to zero as $N \to \infty$ for any $t \le 1$.

   (f) Combine (c)-(e) and derive a numerical method to compute P where A is anti-symmetric and $\|A\| < 1/2$. Construct the algorithm such that the user can specify a tolerance.

   (g) Compare your numerical method with the naive numerical integration approach:

   ```
   P=integral(@(t) expm(t*A')*B*expm(t*A),0,T,'arrayvalued',true);
   ```

   Use $\tau = 1$ and the matrices generated by:

   ```
   A=gallery('neumann',20^2); A=A-A'; A=A/(2*norm(A,1));
   B=sprandn(length(A),length(A),0.05);
   ```

   How much better is the new method?

Connection with current research: In the field of quantum chemistry, the relation (*) for $t = 1$ is commonly called the Baker-Campbell-Hausdorff expansion. It is fundamental in one of the leading numerical methods in that field - the so-called coupled cluster approach.

The quantity P is called a Gramian, and it is often used in system and control in order to study controllability, observability and to derive optimal control as well as carrying out "model order reduction".

Not a part of the exercise: Can you derive a similar algorithm which does not require the matrix to be anti-symmetric?