Theorems sheet Computational Methods of Science

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Definition 1 *A complex matrix A is a normal matrix if $AA^* = A^*A$.*

Theorem 2 *Normal matrices are similar to a diagonal matrix through a unitary transformation.*

Definition 3 (Field of Values) *The field of values of a matrix A is the region in the complex plane given by*

$$F(A) = \{\frac{(x, Ax)}{(x, x)} | x \in C^n \ x \neq 0\}$$

Definition 4 (Generalized Field of Values) *The generalized field of values of a matrix A is the region in the complex plane given by*

$$F_H(A) = \{\frac{(x, HAx)}{(x, Hx)} | x \in C^n; \ x \neq 0\}$$

where H is positive definite, but not necessarily Hermitian.

Theorem 5 $\sigma(A) \subset F(A)$ *and* $\sigma(A) \subset F_H(A)$

Theorem 6 *If A or $P^{-1}AP$ is normal then the convex hull of $\sigma(A)$ is $F(A)$ or convex hull of $\sigma(A)$ is $F_{(PP^T)^{-1}}(A)$, respectively.*

Theorem 7 *Any matrix can be split in a Hermitian and a skew Hermitian part: $A = (A + A^*)/2 + (A - A^*)/2$, here the first term is Hermitian and the second skew Hermitian.*

Theorem 8 *$F_{(A+A^*)/2}$ is real and $\min(\sigma((A + A^*)/2)) \leq F_{(A+A^*)/2} \leq \max(\sigma((A + A^*)/2))$. Likewise the Field of Values of the skew symmetric part is purely imaginary and it holds that $\min(imag(\sigma((A - A^*)/2))) \leq imag(F_{(A-A^*)/2}) \leq \max(imag(\sigma((A - A^*)/2)))$.*

Theorem 9 (Alternative Bendixon) *$F_A \subseteq (F_{(A+A^*)/2} + F_{(A-A^*)/2})$, hence $\sigma(A)$ in the rectangle defined by the two corners $(\min(\sigma((A + A^*)/2)), i\min(imag(\sigma((A - A^*)/2)))$ and $(\max(\sigma((A + A^*)/2)), i\max(imag(\sigma((A - A^*)/2)))$*

Theorem 10 *If A is real then if (λ, x) is an eigenpair then also $(\bar{\lambda}, \bar{x})$ is an eigenpair. Hence , $\min(imag(\sigma((A - A^*)/2))) = -\max(imag(\sigma((A - A^*)/2)))$.*

Theorem 11 *If A is positive definite then also S^TAS is positive definite for any nonsingular S, and moreover, any matrix that is similar to S^TAS has its spectrum in the positive half plane.*

Corollary 12 *In particular $\sigma(SS^TA) > 0$, hence $\sigma(HA) > 0$ for any SPD matrix H.*

Theorem 13 *Any real irreducible tridiagonal matrix A is similar to a tridiagonal matrix B with* $a_{i,i-1}a_{i-1,i} = b_{i,i-1}b_{i-1,i}$ *for* $i = 2, \cdots, n$ *such that* $|b_{i,i-1}| = |b_{i-1,i}|$. *The transformation matrix is real and diagonal.*

Corollary 14
1. *If additionally the matrix A has positive off diagonal elements then it is similar to a symmetric matrix B.*
2. *If the matrix A has a zero diagonal part and* $sign(a_{i,i-1}) = -sign(a_{i-1,i})$ *for* $i = 1, \cdots, n$, *then it is similar to a skew symmetric matrix.*

Theorem 15 *If* $u_n = Au_{n-1}$, $\rho(A) \leq 1$ *and* $P^{-1}AP$ *is normal then* $||u_n||_2 \leq \kappa_2(P)||u_0||_2$, *where* $\kappa_2(P) \equiv ||P||_2||P^{-1}||_2$ *is the condition number of P.*

Theorem 16 *If* $\frac{d}{dt}u = Au$, $\sigma(A) \leq 0$ *and* $P^{-1}AP$ *is normal then* $||u(t)||_2 \leq \kappa_2(P)||u(0)||_2$, *where* $\kappa_2(P) \equiv ||P||_2||P^{-1}||_2$ *is the condition number of P.*

Definition 17 (Non-negativeness) *A matrix A is non-negative* $(A \geq 0)$ *if each element is non negative, and A is positive* $(A > 0)$ *if each element is positive.*

Definition 18 (Monotony) *A matrix A is monotone if its inverse exists and is non-negative*

Theorem 19 *A matrix A is monotone if and only if from* $Ax \geq 0$ *it follows that* $x \geq 0$.

Definition 20 (M-matrix) *A matrix A is an M-matrix if A is monotone and* $a_{ij} \leq 0$ $(\forall i \neq j)$.

Theorem 21 *An M-matrix has positive diagonal elements.*

Theorem 22 *An irreducible, weakly diagonally dominant matrix A with positive diagonal elements and* $a_{ij} \leq 0$ $(\forall i \neq j)$ *is an M-matrix.*

Theorem 23 *If* J_i *is a Jordan block of order p, then it holds for* $n \to \infty$

$$||J_i^n|| \approx cn^{p-1}|\lambda_i|^n$$

where c is a constant that depends on the choice of the norm.

Tentamen Computational Methods of Science
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Duration: 3 hours.

In front of the questions one finds the weights used to determine the final mark.

Problem 1

a. [3] Bring the following equations defined on [0,1] and $t \geq 0$ to diagonal form and determine where and which boundary conditions have to be applied (assume that $u(x,0)$ and $v(x,0)$ are given):

$$\begin{aligned} u_t &= 2u_x - v_x \\ v_t &= -u_x + 2v_x \end{aligned}$$

b. [3] Given the symmetric bilinear form $(Du, Dv)_h$ with $(Du)_i = (u_i - u_{i-1})/h$ for $i = 1, ..., n$ with $h = 1/n$ on the space R^{n+1} where $u_0 = 0$ and $(u, v)_h = h \sum_{i=1}^{n} u_i v_i$. Which selfadjoint difference operator is attached to this bilinear form? Give field and boundary operator separately. To which continuous operators are these discrete operators approximations?

c. [2] Which steps have to be taken to simulate a physical field problem, that can be represented by a PDE, on a computer in such a way that the results are reliable approximations to the physics?

Problem 2

Consider the convection diffusion problem $u_t = -\nu u_x + \mu u_{xx}$, $\mu, \nu \geq 0$ on the interval $[0, 1]$ and $t > 0$ with $u(x, 0)$, $u(0, t)$ and $u(1, t)$ given.

a. [2] Use central differences on a uniform mesh with $m + 1$ grid points, i.e. constant mesh size $\Delta x = 1/(m + 1)$, to discretize u_x and u_{xx} and show that we end up with a system of ODEs of the form

$$\frac{d}{dt}u = \nu Cu + \mu Du + f(t) \tag{1}$$

which is a second-order approximation to the original PDE. Here, C is a skew-symmetric matrix and D a symmetric matrix, following from the discretization of the first and second derivative, respectively. Both matrices will be tridiagonal with coefficients that are constant along a diagonal. Give, C,D and $f(t)$.

b. [3] Show that C and D are normal matrices but $\nu C + \mu D$ in general is not. Next, using the Alternative Bendixon theorem (Th. 9 from sheet), Gerschgorin's theorem and Taussky's theorm, sketch the rectangle in the complex plane where the eigenvalues of $\nu C + \mu D$ are located. Can the matrix become singular?

Exam questions continue on other side

c. [3] Suppose one applies the Trapezoidal method to the system of ODEs (1). Moreover suppose that we study the growth of an initial perturbation, show that we end up with an expression $e^{(n+1)} = Ae^{(n)}$ where A is a rational expression in the Jacobian of the right-hand side of (1). Show that A is unitary if $\mu = 0$ and consequently that $||e^{(n)}||_2 = ||e^{(0)}||_2$. Show that for $\nu = 0$ the matrix A is normal and consequently that $||e^{(n)}||_2 \leq ||e^{(0)}||_2$.

d. [2] For which ratio μ/ν is the matrix $\nu C + \mu D$ reducible. In this case, is it possible to make the matrix normal by a similarity transformation, and why?

e. [2] Suppose we apply the forward Euler method to (1) where the ratio is given in previous part. Again we write it in the form $e^{(n+1)} = Ae^{(n)}$. Compute the time step for which the eigenvalues of A are all minus one. What can be said about the behavior of $||A^n||$ in this case? Is there also a dependency on m (for m see part a)?

f. [2] For the irreducible case, the matrix $\nu C + \mu D$ is similar to a normal matrix by means of a similarity transformation using a diagonal matrix with positive entries (see Th. 13 and Corol. 14 from Form. sheet). Sketch for the obtained normal matrix the domain in the complex plane where the eigenvalues are located. Distinguish two cases (i) the off diagonal elements have the same sign, and (ii) the elements on the upper diagonal have signs opposite to those on the lower diagonal.

g. [2] In order to estimate the possible growth in the irreducible case using the transformation performed in the previous part, compute the diagonal matrix which makes the matrix $\nu C + \mu D$ normal. For this, set this diagonal matrix $H = \text{diag}(1, h_2, h_3, ..., h_m)$, derive an expression for h_{i+1}/h_i and compute h_i. Applying the Trapezoidal method to (1), bound $||e^{(n)}||_2$ in $||e^{(0)}||_2$, where it is given that the two-norm of a diagonal matrix is just the maximum element in absolute value,

Problem 3

a. [3] Suppose A is an SPD matrix and we want to solve $Ax = b$. Which minimization problem over a subspace $\mathcal{V}$ is associated to this problem? Show that the minimization leads to the same approximation as the one obtained from a Galerkin approximation of $Ax = b$ on $\mathcal{V}$. What is the connection of this to the CG method? And for which norm the error is monotonically decreasing in the CG method?

b. [3] Show that a Krylov subspace is shift-invariant. Show that once an eigenvector is in the subspace then it is found in the Arnoldi method. Suppose the eigenvalues of a real symmetric matrix or order n are just $1, 2, ..., n$ and all associated eigenvectors are occurring with an equal weight in the initial guess. Which eigenvalues will converge first in the Arnoldi method? Also give a lower bound to the convergence speed using the connection with the power method.