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2D1266, Mathematical models, Analysis and Simulation, part I
Monday Dec 17th 2001, 14-19

Closed book examination 5 hours. A sum of credits of 50, homework included, is certainly enough to pass. The results will be announced no later than January 7th.

P1. Given the linear system of equations $Ax = b$, where

$$A = \begin{pmatrix} 4 & -2 & -2 & -2 \\ -2 & 5 & 0 & 0 \\ -2 & 0 & 5 & 0 \\ -2 & 0 & 0 & 10 \end{pmatrix}$$

a) (3) Find the LDL^T-factorization of A. Is A positive definite or positive semi-definite?

b) (2) With help of the LDL^T find the Cholesky-factorization of A.

c) (4) Incomplete Cholesky-factorization means that $A = \tilde{L}\tilde{L}^T - E$, where $\tilde{L}$ has the same sparsity pattern as the lower triangular part of A. Find $\tilde{L}$ and E.

P2. A is a real symmetric $n \times n$ matrix with eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. The following iterative scheme is used for solving $Ax = b$.

$$x_{k+1} = x_k - \alpha r_k, \quad r_k = Ax_k - b$$

Let $e_k = A^{-1}b - x_k$ and $\kappa = \lambda_n/\lambda_1$, the condition number of A.

a) (3) Show that $e_{k+1} = Be_k$ with $B = I - \alpha A$. What are the eigenvalues of B?

b) (3) Show that

$$\frac{e_{k+1}^T e_{k+1}}{e_k^T e_k} \leq \max_k (1 - \alpha\lambda_k)^2$$

c) (4) Show that one can choose α such that

$$\|e_{k+1}\|_2 \leq \frac{\kappa - 1}{\kappa + 1}\|e_k\|_2$$

P3. a) (3) Find the critical points of the differential equation

$$\frac{dx}{dt} = x - x^3$$

Investigate if they are stable or unstable. Sketch trajectories in the $(t, x) - plane$ of the solutions with starting values $x(0) = -2, -\epsilon, +\epsilon$ and 2, where $0 < \epsilon << 1$.

b) (3) Find the critical points of the differential equation

$$\frac{d^2x}{dt^2} = x - x^3$$

Investigate if they are stable or unstable. Give a sketch of the phase-portrait in the vicinity of the critical points.

P4. Given the boundary value problem

$$-\frac{d^2u}{dx^2} + u = f(x), \quad u(0) = 0, \quad \frac{du}{dx}(1) = 0$$

a) (3) In the weak form (variational form) formulation: Find $u \in V$ such that

$$a(u, v) = L(v), \qquad for \quad all \quad v \in V$$

specify the bilinear form $a(u, v)$, the functional $L(v)$ and the function space V.

b) (3) In the Galerkin method formulation of the problem: Find $u_h \in V$ such that

$$a(u_h, v) = L(v), \qquad for \quad all \quad v \in V_h$$

describe the function space V_h in case V_h consists of "roof" functions defined on an equidistant grid on $[0, 1]$. If the stepsize h is $h = 1/2$, how does the ansatzfunction look like? What is the dimension of the matrix A assiciated with $a(u_h, v)$?

P5. A simple chemical reaction network is the system

If x_1, x_2, x_3 denotes the concentrations of A, B, C the following system of ODE's models the kinetic behaviour of the species

$$\frac{dx}{dt} = \begin{pmatrix} -k_{12} - k_{13} & k_{21} & k_{31} \\ k_{12} & -k_{21} - k_{23} & k_{32} \\ k_{13} & k_{23} & -k_{32} - k_{31} \end{pmatrix} x \quad (*)$$

The rate constants k_{ij} are all positive quantities. The components of the solution vector $x(t)$ fullfils a positivity property: $x_i(t) > 0$ for all $t > 0$ if the components of the initial vector $x(0)$ are nonnegative (you need not show that).

a) (2) What are the critical points of $(*)$?

b) (2) If $x(0) = (1, 0, 0)^T$ is given, show that $x_1(t) + x_2(t) + x_3(t) = 1$ for all $t \geq 0$.

c) (3) The relation in b) states that the solutions dwell in a plane in R^3. Let the equilibrium point X be the critical point associated with the initial vector $(1, 0, 0)^T$. The solution can be written $x(t) = X + Uy(t)$, where U is a 3×2-matrix. Find an orthogonal matrix U and formulate the corresponding ODE-system for $y(t)$.

d) (4) The equilibrium point is always stable, but the approach to equilibrium can be oscillatory (spirals in the phase portrait) depending on the values of the rate constants. This behaviour is not correct from thermodynamic point of view, the approach to equilibrium should be exponential, i.e.

$$X = \lim_{t \to \infty} (X + \sum c_i e^{-\mu_i t})$$

Show that with the extra condition that all three reactions are in balance, i.e.

$$k_{12}X_1 = k_{21}X_2, \qquad k_{23}X_2 = k_{32}X_3, \qquad k_{31}X_3 = k_{13}X_1$$

the approach to equilibrium will be exponential.
Hint: Use a transformation $x(t) = X + Dz(t)$, where D is a 3×3 diagonal matrix. Try to choose the elements in D so that a symmetric matrix is obtained.

P6 (5). Fomulate the upwind method for the first order wave equation

$$u_t = cu_x, \quad u(x,0) = u_0(x)$$

where c is a positive constant and u_0 is the given initial data. Show that the von Neumann stbility criterion is satisfied if

$$0 < c\frac{\Delta t}{\Delta x} \leq 1$$

P7. Given a set of measurement points (t_i, x_i), $\quad i = 1, 2, \ldots m$ and a mathematical model $x(t) = \sum_{j=1}^{n} c_j \varphi_j(t), m >> n$. We want to fit the model to the given data in the weighted linear least squares sense, i.e. find the vector c solving the minimization problem

$$\min_c F(c), \quad where \quad F(c) = \sum_{i=1}^{m} w_i (x(t_i) - x_i)^2 \quad (*)$$

a) (1) Formulate with a matrix the overdetermined system of linear equations which is obtained for $x(t_i) \approx x_i, i = 1, 2, \ldots, m$.

b) (2) Multiply both sides in the system in a) with a suitable matrix W with elements being functions of $w_i, i = 1, 2, \ldots, m$. The sum of the squares of the residuals of this system should be identical to the function $F(c)$ in $(*)$.

c) (3) Give the matrix P in the solution formula $c = Px$. P ia a function of the matrix in a) and the matrix W in b).