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WT 2002/2003

Introduction to Scientific Computing

Mid-Term Exam, December 19th 2002

Name: ______________________________

- The exam consists of four problems and is divided into two parts:
  - The first part (problems 1 and 2) is without materials like notes, books etc. at all. You will have 50 minutes for this part.
  - For the second part (problems 3 and 4), you may books, lecture notes etc., but no electrical devices like for example calculators, mobile phones, ... You will have 40 minutes for this part.

  You have to hand in your answers for part one before you receive the second part of the questions and may start using media.
- Part one consists of three pages (in addition to this page), part two is on pages 5-7. Please check your copy for comleteness!
- The level of difficulty of the questions is quite different, and we did not sort them according top difficulty. Therefor, if you have problems with some question, just proceed to the next part before loosing too much time.

1 General questions

a) Which are the two main steps of modelling? *(2 points)*

  - *derivation*
  - *analysis*

b) Imagine you want to modell a chemical reactor. Name four basic questions you have to answer to derive an appropriate model (thinking about simulation in general, not only about your reactor)! *(4 points)*

- *What is the task of the model (optimization, insight, ...)?*
- *What is the required level of detail (resolution, dimensions, ...)?*
- *Which quantities are important and how important are they?*
- *What are their relations and interactions?*

c) Name three general questions you have to answer if you analyse a model! *(3 points)*

- *Existence of a solution?*
- *Uniquness of the solution?*
- *Robustness of the model with respect to the input data/condition of the equations?*

d) Name four possible ways to solve/simulate a model (each of them not applicable for all types of models)! *(4 points)*

- *Try and error,*
- *analytical solution,*
- *direct numerical solution,*
- *approximative numerical solution.*

2 Continuous Models: ODE and PDE

$$\dot{p}(t) = a \cdot p(t), \quad p(0) = p_0, \tag{1}$$
$$\dot{q}(t) = b \cdot q(t), \quad q(0) = q_0, \tag{2}$$

$$a, b > 0.$$

Consider the above ODEs for the growth of the population p and q of two species P and Q.

a) Describe the behaviour of p for t tending to infinity. Is this behaviour realistic? *(3 points)*

The exact solution of equation (1) is

$$p(t) = p_0 \cdot e^{a \cdot t}.$$

Thus,

$$\lim_{t \to \infty} p(t) = \infty.$$

This behaviour is not realistic as at some point, e. g. lack of nutrients will prevent further growth of population.

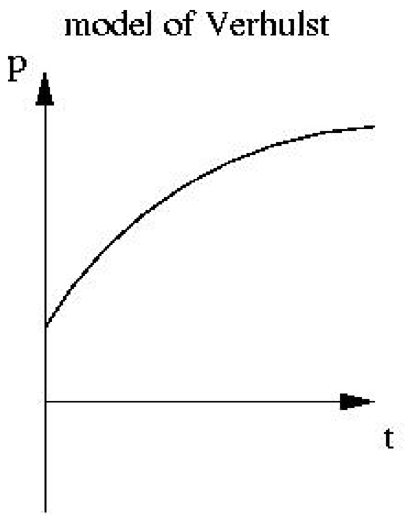
b) Give two possible variations of equation (1) with a more realistic behaviour for t tending to infinity (but still without interactions of the two species). For both possiblities, draw the qualitative behaviour of the resulting population p in the diagrams below. *(4 points)*

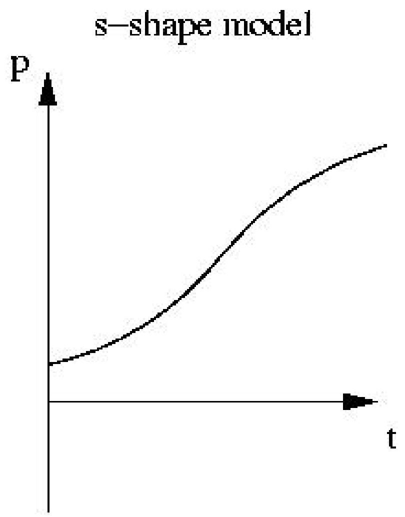
Model of Verhulst (linear decrease of population growth):

$$\dot{p}(t) = a - b \cdot p(t), \quad a, b > 0$$

S-shape growth (postive linear and negative quadratic part of the growth rate per time unit):

$$\dot{p}(t) = a \cdot p(t) - b \cdot p^2(t), \quad a, b > 0.$$





c) Why are linear ODEs not sufficient to model the s-shape form of the population curve, which can be observed for real world populations? *(2 points)*

A necessary condition for the s-shape is a change of sign of the second derivative. For a general linear ODE $\dot{p} = a \cdot p + b$, we get

$$\ddot{p} = a \cdot \dot{p}.$$

Thus, a change of sign of the second derivative nonnegative growth rates $\dot{p}$ at the same time is impossible.

d) To include interactions of the two species in the above model, add suitable terms that model the following assumtion:

The decrease of population p per time unit is proportional to the number q of individuals of species Q (and vice versa for q). *(1 point)*

$$\begin{aligned}\dot{p}(t) &= a \cdot p(t) - c \cdot q(t), c > 0,\\ \dot{q}(t) &= b \cdot q(t) - d \cdot p(t), d > 0\end{aligned}$$

e) Is there an equilibrium $\bar{p}, \bar{q} > 0$ for the system of ODEs from d)? *(4 points)*

The equilibrium $\begin{pmatrix} \bar{p} \\ \bar{q} \end{pmatrix}$ *is defined by*

$$\begin{aligned}a \cdot \bar{p} - c \cdot \bar{q} &= 0\\ b \cdot \bar{q} - d \cdot \bar{p} &= 0\end{aligned}$$

$$\Leftrightarrow$$

$$\begin{pmatrix} a & -c \\ b & -d \end{pmatrix} \begin{pmatrix} \bar{p} \\ \bar{q} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Gaußian elimination:

$$\begin{pmatrix} a & -c \\ 0 & -d + \frac{c}{a} b \end{pmatrix} \begin{pmatrix} \bar{p} \\ \bar{q} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

$$\Leftrightarrow$$

$$\bar{p} = \bar{q} = 0, \text{ if } -d + \frac{c}{a} b \neq 0,$$

$$\bar{p} = \frac{c}{a} \bar{q}, \bar{q} \in |R.$$

Thus, there is an infinite number of equlibria with $\bar{p}, \bar{q} > 0$.

f) Consider the original ODE (1) for p. We now assume that the population p depends on time t *and* the position x ($x \in [0; 1]$) on an east-west axis. Enhance the above model for p according to the following assumptions:

1) The growth per time unit and individual is proportional to x. *(1 point)*

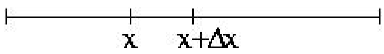
2) The movement of people to neighbouring locations is proportional to the negative steepness of p in the respective directions (thus, people move to regions with a less dense poulation).

Hint: Imagine a small interval on the x-axis and compute the change of population within this interval from the movement of people over both borders of the interval. Compute the limit for the interval length tending to zero. *(3 points)*

1) The growth per time unit and individual is desribed mathematically by $\frac{\dot{p}(t)}{p(t)}$*. Thus, the modified equation is*

$$p_t(x,t) = a \cdot x \cdot p(x,t).$$

2) We look at an interval with legth Δx *on the* x*-axis:*



On the lefthand side of the interval, the steepness of p from the left to right is given by $p_x(x)$*. Analoguously, on the righthand side of the interval, the steepness from the right to the left is* $-p_x(x+\Delta x)$*. Thus, the change of population per time unit within the interval is*

$$p_x(x+\Delta x) - p_x(x).$$

The average change per point on the x-axis is proportional to

$$\frac{p_x(x+\Delta x) - p_x(x)}{\Delta x}.$$

Establishing the limit $\Delta x \to 0$*, we get the additional term* p_{xx} *for the growth per time unit. Thus, the modified equation is*

$$p_t(x,t) = a \cdot p(x,t) + b \cdot p_{xx}(x,t), b > 0.$$

3 Numerical Methods for ODE

Consider the first-order ODE

$$\dot{y} = f(y,t), \quad y(0) = y_0.$$

Derive a pth-order discretization on an equidistant grid

$$\{t_i = i * h; i = 1, 2, 3, \ldots \& h > 0\}$$

a) for $p = 2$ using Taylor-expansion of $y(t_{k+1})$ with respect to $y(t_k)$, *(3 points)*

$$y(t_{k+1}) = y(t_k) + h \cdot \dot{y}(t_k) + \frac{h^2}{2} \cdot \ddot{y}(t_k) + \frac{h^3}{6} \cdot \dddot{y}(t_k) + O(h^4).$$

The derivatives of y can be expressed with the help of f:

$$\begin{aligned}
\dot{y}(t_k) &= f(y(t_k), t_k) \\
\ddot{y}(t_k) &= f_t(y(t_k), t_k) + f_y(y(t_k), t_k) \cdot \dot{y}(t_k) \\
&= f_t(y(t_k), t_k) + f_y(y(t_k), t_k) \cdot f(y(t_k), t_k).
\end{aligned}$$

Thus, the second-order discretization derived from Taylor-expansion is

$$y_{k+1} = y_k + h \cdot f(y_k, t_k) + \frac{h^2}{2} \cdot (f_t(y_k, z_k) + f_y(y_k, t_k) \cdot f(y_k, t_k)).$$

b) for $p = 3$ according to the Adams-Bashforth-approach. *(7 points)*

Replace f in the integral form

$$y(t_{k+1}) - y(t_k) = \int_{t_k}^{t_{k+1}} f(y(t), t)\, dt$$

by the interpolating polynomial with degree 2 with interpolation points (y_{k-1}, t_{k-1}), $(y_{k-1}, t_{k-1}), (y_k, t_k)$. Using the Lagrange polynomials, we get:

$$p(t) = f(y_{k-2}, t_{k-2}) \cdot L_0(t) + f(y_{k-1}, t_{k-1}) \cdot L_1(t) + f(y_k, t_k) \cdot L_2(t),$$

where $l_i, i = 0, 1, 2$ are polynomials with

$$L_i(t_{k-2+j}) = \delta_{i,j} = \begin{cases} 1, & \textit{if } i = j, \\ 0 & \textit{else} \end{cases} .$$

$\Rightarrow$

$$\begin{aligned}
L_0(t) &= \frac{(t - t_{k-1})(t - t_k)}{(t_{k-2} - t_{k-1})(t_{k-2} - t_k)}, \\
L_1(t) &= \frac{(t - t_{k-2})(t - t_k)}{(t_{k-1} - t_{k-2})(t_{k-1} - t_k)}, \\
L_2(t) &= \frac{(t - t_{k-2})(t - t_{k-1})}{(t_k - t_{k-2})(t_k - t_{k-1})}.
\end{aligned}$$

$\Rightarrow$

$$\begin{aligned}
L_0(t_k+T) &= \frac{1}{2h^2}(T+h)T = \frac{1}{2h^2}(T^2+hT),\\
L_1(t_k+T) &= \frac{1}{-h^2}(T+2h)T = -\frac{1}{h^2}(T^2+2hT),\\
L_2(t_k+T) &= \frac{1}{2h^2}(T+2h)(T+h) = \frac{1}{2h^2}(T^2+3hT+2h^2).
\end{aligned}$$

$$\begin{aligned}
\int_{t_k}^{t_{k+1}} L_0(t)\,dt &= \int_0^h L_0(t_k+T)\,dT = \frac{1}{2h^2}\int_0^h T^2+hT\,dT\\
&= \frac{1}{2h^2}\left[\frac{T^3}{3}+\frac{hT^2}{2}\right]_0^h = \frac{5}{12}h\\
\int_{t_k}^{t_{k+1}} L_1(t)\,dt &= \int_0^h L_1(t_k+T)\,dT = -\frac{1}{h^2}\int_0^h T^2+2hT\,dT\\
&= -\frac{1}{h^2}\left[\frac{T^3}{3}+hT^2\right]_0^h = -\frac{4}{3}h\\
\int_{t_k}^{t_{k+1}} L_2(t)\,dt &= \int_0^h L_2(t_k+T)\,dT = \frac{1}{2h^2}\int_0^h T^2+3hT+2h^2\,dT\\
&= \frac{1}{2h^2}\left[\frac{T^3}{3}+\frac{3hT^2}{2}+2h^2T\right]_0^h = \frac{23}{12}h.
\end{aligned}$$

$$\Rightarrow y_{k+1} = y_k + \frac{h}{12}\cdot\left(5f(y_{k-1},t_{k-1}) - 16f(y_{k-1},t_{k-1}) + 23f(y_k,t_k)\right).$$

4) Numerical Methods for PDE

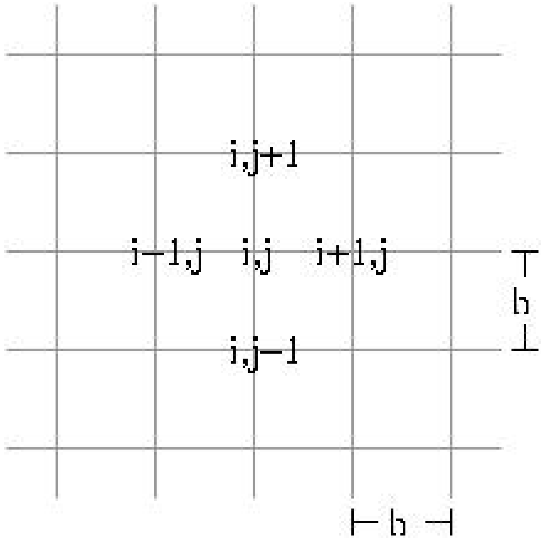
Consider the Poisson equation

$$\Delta u = f \quad \text{in} \quad]0;1[^2$$

with boundary conditions

$$p = 0 \quad \text{at} \quad \{0\}\times[0;1]\cup\{1\}\times[0;1]\cup[0;1]\times\{0\}\cup[0;1]\times\{1\}$$

and the following finite-difference discretization on a square grid:



$$\Delta u(x_{i,j}) \approx \frac{u_{i-1,j-1} + u_{i-1,j+1} - 4u_{i,j} + u_{i+1,j-1} + u_{i+1,j+1}}{2h^2}$$

at all inner grid points $x_{i,j}$.

Is this discretization

a) consistent, *(6 points)*

Taylor-expansion of u *with respect to* $x_{i,j}$*:*

$$\begin{aligned}
u(x_{i+1,j+1}) &= u(x_{i,j}) + h \cdot (u_{x_1}(x_{i,j}) + u_{x_2}(x_{i,j})) + \\
&\quad \frac{h^2}{2}(u_{x_1x_1}(x_{i,j}) + 2u_{x_1x_2}(x_{i,j}) + u_{x_2x_2}(x_{i,j})) + O(h^3), \\
u(x_{i-1,j+1}) &= u(x_{i,j}) + h \cdot (-u_{x_1}(x_{i,j}) + u_{x_2}(x_{i,j})) + \\
&\quad \frac{h^2}{2}(u_{x_1x_1}(x_{i,j}) - 2u_{x_1x_2}(x_{i,j}) + u_{x_2x_2}(x_{i,j})) + O(h^3), \\
u(x_{i+1,j-1}) &= u(x_{i,j}) + h \cdot (u_{x_1}(x_{i,j}) - u_{x_2}(x_{i,j})) + \\
&\quad \frac{h^2}{2}(u_{x_1x_1}(x_{i,j}) - 2u_{x_1x_2}(x_{i,j}) + u_{x_2x_2}(x_{i,j})) + O(h^3), \\
u(x_{i-1,j-1}) &= u(x_{i,j}) + h \cdot (-u_{x_1}(x_{i,j}) - u_{x_2}(x_{i,j})) + \\
&\quad \frac{h^2}{2}(u_{x_1x_1}(x_{i,j}) + 2u_{x_1x_2}(x_{i,j}) + u_{x_2x_2}(x_{i,j})) + O(h^3).
\end{aligned}$$

$$\Rightarrow \quad u(x_{i+1,j+1}) + u(x_{i-1,j+1}) + u(x_{i+1,j-1}) + u(x_{i-1,j-1}) = \\
4(u(x_{i,j}) + \frac{h^2}{2}(u_{x_1x_1}(x_{i,j}) + u_{x_2x_2}(x_{i,j}))) + O(h^3).$$

$$\Rightarrow \quad \Delta u(x_{i,j}) - \frac{u(x_{i-1,j-1}) + u(x_{i-1,j+1}) - 4u(x_{i,j}) + u(x_{i+1,j-1}) + u(x_{i+1,j+1})}{2h^2} =$$

$O(h) \to 0$ *for* $h \to 0$.

$\Rightarrow$ *The discretization is consistent.*

b) stable (hint: try to find an oscillating pattern in the following cutaway of the grid with boundary zero that is annihilated by the discrete operator), *(2 points)*

1	0	1	0	1
0	1	0	1	0
1	0	1	0	1
0	1	0	1	0
1	0	1	0	1

As there is an oscillating pattern, which is annihilated by the operator and fulfilling the boundary conditions, the discretization is instable.

c) convergent? *(1 point)*

As shown in b), the discretization is instable. Thus, it is not convergent as for arbitrarily small h, arbitrarily high oszillations can occur.

Give short reasons for your answers.