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Numerical Optimization with Differential Equations 1 - WS 2018/2019

Exercise 6

Exercise 1

We want to find a line

$$x(t,p) = p_1 + p_2 t$$

to the measurement data

t_i	-2	-1	0	1	2
η_i	0.5	0.5	2	3.5	3.5

such that

$$F(p_1,p_2) = \sum_i (x(t_i,p) - \eta_i)^2$$

is minimal. Determine the optimal parameter $p^* = (p_1^*, p_2^*)$ using the Moore-Penrose Inverse.

(4 Points)

Exercise M4

We consider again the predator-prey system from the previous exercises with the initial values

$$\alpha = 0.2,\ \beta = 0.01,\ \gamma = 0.001,\ \delta = 0.1$$
$$R(0) = 10,\ B(0) = 20.$$

a) Solve the initial value problem for $t = [0, 100]$ and generate equidistant synthetic measurements $\eta_i = x(t_i) + \varepsilon_i$ for $t_i = 5i,\ i = 0,\dots,20$ with Gaussian measurement noise ε_i with standard deviation 5 (which can be generated by `5*randn(2,21)`).

b)
- Write a function `[F, J] = lotka_lsqfunc(x0p, t, eta)` which computes the non-linear function

$$F(x^0,p) = \begin{pmatrix} x(t_0; x^0, p) - \eta_0 \\ \vdots \\ x(t_{20}; x^0, p) - \eta_{20} \end{pmatrix} \in \mathbb{R}^{42},$$

  where $x(t; x^0, p)$ denotes the solution of the initial value problem with initial values x^0 and parameters p evaluated at time t. In addition, the function should return the Jacobian $J(x^0,p)$ of $F(x^0,p)$ with respect to x^0 and p. You should base your computation of J on the VDE approach of exercise M3.
- Use the SVD of J to compute 10 Gauss-Newton steps for the problem

$$\min_{x^0\in\mathbb{R}^2, p\in\mathbb{R}^4} \|F(x^0,p)\|_2,$$

  starting from the exact initial guess $x^0 = (20,10)^T,\ p = (0.2, 0.01, 0.001, 0.1)^T$.

c) 1. Write a function `[F1, F2, J1, J2] = lotka_clsqfunc(sp, t, eta)` which computes the nonlinear functions

$$F_1(s^0,\dots,s^{20},p) = \begin{pmatrix} s^0 - \eta_0 \\ \vdots \\ s^{20} - \eta_{20} \end{pmatrix} \in \mathbb{R}^{42},\ F_2(s^0,\dots,s^{20},p) = \begin{pmatrix} x(t_1;t_0,s^0,p) - s^1 \\ \vdots \\ x(t_{20};t_{19},s^{19},p) - s^{20} \end{pmatrix} \in \mathbb{R}^{40}$$

where additional multiple shooting variables $s^l \in \mathbb{R}^2$, $l = 0,\dots,20$, are used at each measurement time t^l and where $x(t;\tau_0,x^0,p)$ denotes the solution of the initial value problem evaluated at time t with initial values x^0 and τ_0 and parameters p. In addition, the function should return the Jacobians J_1 and J_2 with respect to $s^0,\dots,s^{20}$, and p of F_1 and F_2, respectively. You should base your computation of J_2 on the VDE approach of exercise M3.

2. In order to solve the constrained nonlinear least-squares problem

$$\min_{s^0,\dots,s^{20}\in\mathbb{R}^2, p\in\mathbb{R}^4} \frac{1}{2}\|F_2(s^0,\dots,s^{20},p)\|_2^2,$$
$$\text{s.t. } F_2(s^0,\dots,s^{20},p) = 0,$$

compute 10 constrained Gauss-Newton steps using the measurements as initial values for the multiple shooting variables s^l and an initial parameter guess of zero. In order to solve the linearized constrained least-squares subproblems you can use the equivalent form

$$\underbrace{\begin{pmatrix} J_1^T J_1 & J_2^T \\ J_2 & 0 \end{pmatrix}}_{=:K} \begin{pmatrix} \Delta s^0 \\ \vdots \\ \Delta s^{20} \\ \Delta p \\ \hline \Delta\lambda \end{pmatrix} = - \begin{pmatrix} J_1^T F_1 \\ F_2 \end{pmatrix}.$$

You may use the following simplified (but neither very efficient nor very stable) approach:

```
K = [J1'*J1, J2'; J2, zeros(size(J2,1))];
Delta_splambda = K \ [-J1'*F1; -F2];
delta_sp = delta_splambda(1:size(J1,2));
```

Then use `delta_sp` for the step `sp = sp + delta_sp`.

3. Use `spy(K)` to visualize the nonzero pattern of matrix K.

4. Visualize the first five iterates from 2. To this end, each of the five plots should contain the (discontinuous) multiple shooting trajectories of the two states, the values of the shooting variables (marked with $\circ$) and the measurements (marked with $\times$).

(12 Points)

*Hand in solutions on **Tuesday**, December 4th, **at the beginning** of the lecture!*
*Submit your Matlab solutions until **Tuesday**, December 11th, **11:00 AM** by email to your tutor!*