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Numerical Optimization with Differential Equations 1 - WS 2018/2019

Exercise 11

Exercise 1

Let $\alpha, \beta, \gamma \in \mathbb{N}$ and $k \in \mathbb{R}$. A reaction of α units of substance A and β units of substance B into γ units of substance C can be written as

$$\alpha A + \beta B \xrightarrow{k} \gamma C.$$

The integers α, β, γ are called *stoichiometric factors* and k is the reaction rate. We model this chemical reaction with a system of ordinary differential equations that describes the temporal change of the concentrations $[A]$, $[B]$ and $[C]$ according to

$$\frac{d[A]}{dt} = -\alpha k [A]^\alpha [B]^\beta\,, \quad \frac{d[B]}{dt} = -\beta k [A]^\alpha [B]^\beta\,, \quad \frac{d[C]}{dt} = \gamma k [A]^\alpha [B]^\beta.$$

The first equation describes the relation of the reaction rate of A being proportional to the product of $[A]^\alpha$ and $[B]^\beta$, i.e., the concentrations to the power of their respective stoichiometric factors. Every (elementary) reaction consumes α units of A, which leads to the factor $-\alpha$. In general, several reactions happen simultaneously and the concentration changes must be added.

Formulate a system of ordinary differential equations for the system of reactions

$$\begin{aligned} A &\xrightarrow{k_1} B, \\ B + C &\xrightarrow{k_2} A + C, \\ B + B &\xrightarrow{k_3} B + C. \end{aligned}$$

Exercise 2

a) Use the first order necessary optimality conditions to find the extrema of the functions

$$\begin{aligned} f(x,y) &= x^2 + y^2 - xy + 2x - 2y \\ g(x,y) &= x^2 + y^2 - 3xy + 2x - 2y \\ h(x,y) &= x^2 + y^2 - 2xy + 2x - 2y. \end{aligned}$$

b) Check if the found points are local minima of the functions using the second order conditions.

c) Are the found minima also global minima?

Exercise 3
Transfer the forth order system of differential equations

$$v^{(4)}(t) = \ddot{v}(t) - 3w(t)$$
$$w^{(4)}(t) = 11\dot{v}(t)w(t)$$

in a first order system of differential equations.

Exercise 4

Let $J_1 \in \mathbb{R}^{m_1 \times n}$ and $J_2 \in \mathbb{R}^{m_2 \times n}$ be matrices satisfying

- **(CQ)** $\operatorname{Rang}(J_2) = m_2 \leq n$,
- **(PD)** $\operatorname{Rang}\begin{pmatrix} J_1 \\ J_2 \end{pmatrix} = n \leq m_1 + m_2$.

Show

a. The matrix $J_1^T J_1 \in \mathbb{R}^{n \times n}$ is positive definite on the nullspace of J_2, i.e. $x^T J_1^T J_1 x > 0$ for all $x \in \mathbb{R}^n \setminus \{0\}$ with $J_2 x = 0$.

b. The matrix $\begin{pmatrix} J_1^T J_1 & J_2^T \\ J_2 & 0 \end{pmatrix}$ is regular.

Exercise 5
In the lecture you got to know the Mayer and the Lagrange cost functional.

a) Show, that every Mayer cost functional can be transformed into a Lagrange cost functional.

b) Show, that this is also possible in reverse.

Exercise 6
We consider a vehicle propelled by rockets running on a straight track described by the ODE

$$\dot{s}(t) = v(t), \quad \dot{v}(t) = \frac{u(t)}{m(t)} - c_1 v^2(t), \quad \dot{m}(t) = -c_2 u^2(t),$$

where the states s, v, and m denote the position, velocity, and mass of the vehicle and the control u denotes the rocket thrust. The parameters c_1 and c_2 enter in the friction and fuel consumption terms.

(a) Formulate an optimal control problem to save as much fuel as possible when going from $s = 0$ to $s = 10$ within a given time $T > 0$. The initial and terminal velocity must be zero. The initial amount of fuel is $m_0 > 0$.

(b) Discretize the problem from (a) with direct multiple shooting and a piecewise constant control discretization on the shooting grid $0 = t_0 < t_1 < \cdots < t_M = T$. Write down the resulting NLP.

Exercise 7
Consider the problem

$$\begin{aligned} \min_{x_1,x_2} \quad & x_1 + x_2 \\ \text{s.t.} \quad & x_1^2 + x_2^2 - 2 = 0 \end{aligned}$$

Given are $x^0 = (-1,-1)^T$ and $\lambda^0 = -1$.

- Calculate $x^1 = x^0 + \Delta x^0$ using the full step SQP method with the exact Hessian.
- For this purpose, solve the Quadratic Problem in x^0, λ^0.

Exercise 8
Consider for continuously differentiable $F_1 : \mathbb{R}^n \to \mathbb{R}^{m_1}$ and $F_2 : \mathbb{R}^n \to \mathbb{R}^{m_2}$ the constrained nonlinear least-squares problem

$$\begin{aligned} \min_{x} \quad & \tfrac{1}{2}\|F_1(x)\|_2^2 \\ \text{s.t.} \quad & F_2(x) = 0. \end{aligned}$$

Assume that $x^* \in \mathbb{R}^n$ satisfies $F_1(x^*) = 0$ and $F_2(x^*) = 0$ such that [CQ] and [PD] hold in x^*. Show that for constrained Gauß-Newton and arbitrary $\varepsilon > 0$ there exists a neighbourhood of x^* such that the assumptions of the local contraction theorem are satisfied in this neighbourhood with $\kappa \leq \varepsilon$.

You do not have to hand in these exercises, there will be a discussion in the tutorial.