Exercise 1: Nonlinear optimization and numerical optimal control with `CasADi` and IPOPT

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Exercise 1.1

The aim of this exercise is to formulate and solve a simple constrained nonlinear program (NLP) in `CasADi`, as described in the following.

Within a production process, five circles s_i with $i = 1, \ldots, 5$ must be cut out from a square plate with edge size $a = 10$ cm. Three of those circles should have the radius R and two the radius $2R$. The aim is to place the circles on the plate in such way that the radius R can be as large as possible. The center of each circle s_i is expressed in Cartesian coordinates (x_i, y_i). The circles may not lie outside of the plate nor overlap each other. Figure 1 shows a feasible but suboptimal configuration with $R = 1$.
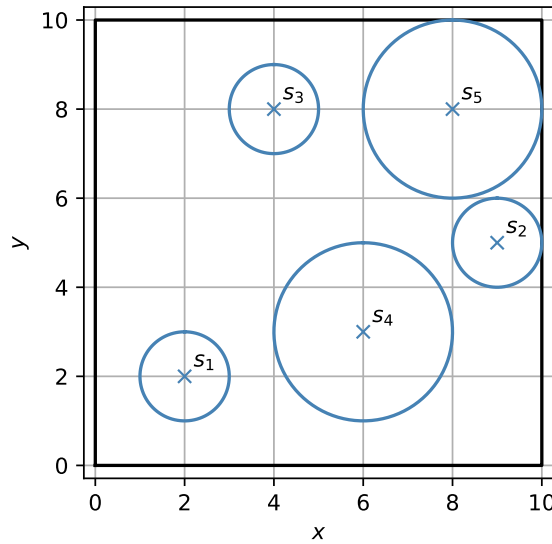

Figure 1: A feasible but suboptimal configuration with $R = 1$.

We can formulate this as the following NLP:

$$\min_{\substack{R, x_1, \ldots, x_5, \\ y_1, \ldots, y_5}} \quad -R \tag{1a}$$

$$\text{s.t.} \quad x_i - r_i(R) \geq 0, \qquad i = 1, ..., 5, \tag{1b}$$

$$x_i + r_i(R) \leq a, \qquad i = 1, ..., 5, \tag{1c}$$

$$y_i - r_i(R) \geq 0, \qquad i = 1, ..., 5, \tag{1d}$$

$$y_i + r_i(R) \leq a, \qquad i = 1, ..., 5, \tag{1e}$$

$$(x_i - x_j)^2 + (y_i - y_j)^2 \geq (r_i + r_j)^2, \qquad i, j = 1, \ldots, 5 \text{ mit } i < j \tag{1f}$$

with $r_i(R) = R$ for $i \in \{1, 2, 3\}$ and $r_i(R) = 2R$ for $i \in \{4, 5\}$.
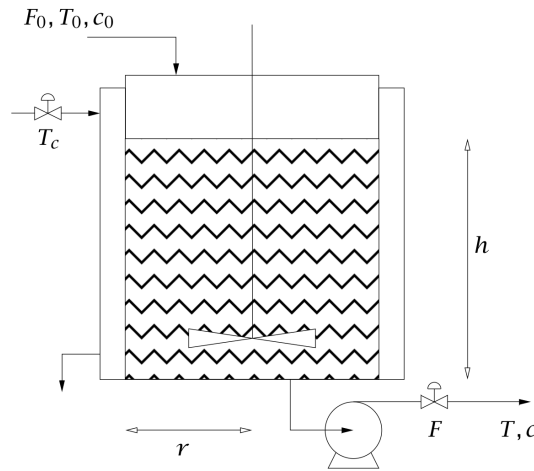
Tasks

1. If you have never before used `CasADi`, take some moments to familiarize yourself with its documentation at https://web.casadi.org/docs/

2. Complete the provided template and run the script in order to solve the problem with `CasADi` and IPOPT. You should see a plot that depicts the positioning of the spheres on the plate, and they should neither overlap nor lie outside the plate. How large is the resulting radius R?

3. In the template, there was already a concrete initialization of the decision variables given. Adapt the initial guess in order to find a better solution, and document the corresponding value of R. What is the best solution you can find?
   Hint: Look at the plot and use your graphical intuition.

4. Check whether the gradient of the Lagrangian is indeed zero at the solution you computed.
   Hint: You might want to find out how `solver.get_function()` works. You can also compute the gradients yourself using `ca.gradient()` or `ca.jacobian()`.

Exercise 1.2

In this exercise, we consider a nonlinear continuous stirred-tank reactor (CSTR).[1]

An irreversible, first-order reaction $A \rightarrow B$ occurs in the liquid phase and the reactor temperature is regulated with external cooling. Mass and energy balances lead to the following nonlinear model:

$$\dot{c} = \frac{F_0(c_0 - c)}{\pi r^2 h} - k_0 \exp\left(-\frac{E}{RT}\right) c,$$

$$\dot{T} = \frac{F_0(T_0 - T)}{\pi r^2 h} - \frac{\Delta H}{\rho C_p} k_0 \exp\left(-\frac{E}{RT}\right) c + \frac{2U}{r \rho C_p}(T_c - T),$$

$$\dot{h} = \frac{F_0 - F}{\pi r^2},$$

with state $x = (c, T, h)$ where c is the concentration of substance A, T is the reactor temperature and h is the height. The controls $u = (T_c, F)$ are the coolant liquid temperature T_c and the outlet flow rate F. Starting from a given initial state $\bar{x}_0$, we want to bring the system into the open loop steady state x^{ref}. We formulate this as the following optimal control problem (OCP):

$$\min_{x_0, u_0, \ldots, u_{N-1}, x_N} \quad \sum_{k=0}^{N-1} l\left(x_k, u_k\right) + l_N(x_N) \tag{2a}$$

$$\text{s.t.} \quad x_0 = \bar{x}_0, \tag{2b}$$

$$x_{k+1} = f(x_k, u_k), \quad k = 0, \ldots, N-1, \tag{2c}$$

$$u_{\min} \le u \le u_{\max}, \quad k = 0, \ldots, N-1, \tag{2d}$$

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[1]The example as well as the figure have been adopted from Example 1.11 in J. B. Rawlings, D. Q. Mayne, and M. M. Diehl. *Model Predictive Control: Theory, Computation, and Design.* Nob Hill, 2nd edition, 2017.

with discrete time horizon N, and where the discrete time dynamics f are obtained by numerical integration of the continuous time dynamics over a time step h using the explicit Runge-Kutta method of fourth order (RK4). The stage and terminal cost are given by

$$l(x_k, u_k) = \frac{1}{2} \left\| x_k - x^{\text{ref}} \right\|_Q^2 + \frac{1}{2} \left\| u_k - u^{\text{ref}} \right\|_R^2, \qquad l_N(x_N) = \frac{1}{2} \| x_k - x^{\text{ref}} \|_P^2. \tag{3}$$

Tasks

1. Complete the provided template and run the script in order to solve the OCP with `CasADi` and IPOPT. Does the resulting trajectory look reasonable and achieve the desired setpoint?

2. Construct the KKT matrix evaluated at the solution, and plot its sparsity pattern. Interpret the resulting block structure. *Hint:* Use `solver.get_function()` and `plt.spy()`. You can also construct it more manually, using, e.g., `ca.hessian()`.