5 Process optimization

5.1 Optimization theory

This section will deal with some basic considerations about optimization theory. It purpose is not an exhaustive review of (convex) optimization but rather to introduce some concepts and terms that will prove useful in the following sections. Foremost a brief discussion of optimality conditions for constrained problems – the so called Karush-Kuhn-Tucker conditions – will be given. Closely linked to those conditions, and in some cases even a perquisite for their validity, are the constraint qualifications which are subsequently discussed.

5.1.1 Karush-Kuhn-Tucker conditions

Considering the most general case of a NLP

introduc active set

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & h_i(x) = 0, \quad i \in \mathcal{E} \\ & g_j(x) \leq 0, \quad j \in \mathcal{I} \end{aligned} \tag{P1}$$

where $f(x) : \mathbb{R}^n \mapsto \mathbb{R}$ denotes the objective function, $\mathcal{E}$ is the set of equality constraints and $\mathcal{I}$ the set of inequality constraints.

The Lagrangian function corresponding to to the problem above can be written as

$$\mathcal{L}(x, \lambda, \mu) := f(x) + \lambda^T h(x) + \mu^T g(x) \tag{5.1}$$

First order KKT conditions must hold at the optimal point (x^*, λ^*, μ^*)

$$\nabla_x \mathcal{L}(x^*, \lambda^*, \mu^*) = 0, \tag{5.2}$$

$$h_i(x^*) = 0, \tag{5.3}$$

$$g_j(x^*) \leq 0, \tag{5.4}$$

$$\mu_j^* \geq 0, \tag{5.5}$$

$$\mu_j^* g_j(x^*) = 0, \tag{5.6}$$

$$i \in \mathcal{E}, \quad j \in \mathcal{I}. \tag{5.7}$$

5.1.2 Constraint qualification conditions

Constraint qualifications, given convexity of the problem, can ensure the existence of strictly positive Lagrange multipliers, such that the unconstrained equivalent problem can be constructed. In general one is interested in the weakest possible perquisite to ensure feasibility of the problem. There are several constraint qualifications proposed in literature, which are differently hard to fulfil and verify.

feasibility the right word here?

Slater's constraint qualification (SCQ)

Among the most widely used constraint qualifications is Slater's constraint qualification

$$\exists \tilde{x}, \forall i \in \mathcal{I} : h_i(\tilde{x}) < 0. \tag{5.8}$$

This qualifications essentially states, that there in fact is a point which will fulfil the constraints.

Linear independence constraint qualification (LICQ)

Another widely used is called the linear independence constraint qualification. It states, given the set of of feasible solutions of the original problem $\mathcal{C} = \{x \in \mathcal{X} \mid h_i(x) \leq 0 \forall i \in \mathcal{I}\}$ and the set of active constraints $\mathcal{A}(\bar{x}) = \{i \in \rangle \mid h_i(\bar{x}) = 0\}$

$$\{\nabla h_i(\bar{x}) \mid i \in \mathcal{A}(\bar{x})\} \qquad \text{is linearly independent.} \tag{5.9}$$

Mangasarian-Fromovitz constraint qualification (MFCQ)

$$\exists \tilde{u}, \forall i \in \mathcal{A}(\bar{x}) : \nabla h_i(\bar{x})(\tilde{u}) < 0. \tag{5.10}$$

5.2 Mixed-integer optimization

In this section some general considerations about mixed-integer non-linear programming (MINLP) will be presented. First the most commonly applied solution techniques will briefly be discussed on the basis of a review on the subject by Grossmann [12]. Then then an alternative approach to solve this class of problems, based on a continuous reformulation of the discrete decision variables, which has recently been proposed [17, 28] will also be introduced. This reformulation is also the basis for a comparison of different approaches to solve this class of problem within the process simulation environment gPROMS®.

5.2.1 Solution techniques

As previously stated, the following discussion of general solution techniques for MINLP's is largely based in the comprehensive review by I. E. Grossmann [12].

Several approaches to tackle this type of problem have successfully been applied to a multitude of cases for several years now. In general four major types of solution algorithms can be distinguished.

- branch and bound
- outer approximation
- generalized benders
- extended cutting plane
- LP/NLP ...

All these algorithms make use of a limited number of common subproblems, which are then solved in different configurations. Therefore these subproblems can previously be discussed and will be referred to when going elaborating on different algorithms. Furthermore it needs to be emphasised, that the presented solution techniques are designed for convex problems, and only in those cases an optimal solution can be found with a degree of confidence. While they can be applied to the more general non-convex case, only local optimality can be assured.

The general case of a MINLP takes the form

$$\begin{aligned} \min_{x,y} \quad & C = f(x,y) \\ \text{s.t.} \quad & g_j(x,y) \leq 0, \;\; j \in \mathcal{J} \\ & x \in \mathcal{X}, \;\; y \in \mathcal{Y} \end{aligned} \tag{P2}$$

If the discrete variables in the discrete-continuous program are relaxed, the resulting NLP relaxation can be written as

$$\begin{aligned} \min_{x,y} \quad & C^k_{LB} = f(x,y) \\ \text{s.t.} \quad & g_j(x,y) \leq 0, \;\; j \in \mathcal{J} \\ & x \in \mathcal{X}, \;\; y \in \mathcal{Y}_R \\ & y_i \leq \alpha^k_i, \;\; i \in \mathcal{I}^k_{FL} \\ & y_i \geq \beta^k_i, \;\; i \in \mathcal{I}^k_{FU} \end{aligned} \tag{P3}$$

Here $\mathcal{Y}_R$ denotes the relaxed set of the integer set $\mathcal{Y}$, $\mathcal{I}^k_{FL}$ and $\mathcal{I}^k_{FU}$ are subsets of the indices denoting the entire set of integer variables. The relaxed integers contained in these sets are bounded to the values α^k_i and β^k_i respectively. These bounds are lower and upper bound taken from the previous iteration of the algorithm in question. If $\mathcal{I}^k_{FL} = \emptyset$ and $\mathcal{I}^k_{FU} = \emptyset$ are empty sets, problem (P3) denotes the fully relaxed problem, initially solved in all algorithms. The optimal solution to this initially solved problem (C^0_{LB}) poses an absolute lower bound to (P2) since all variables are fully relaxed.

If all discrete variables are fixed at a given value, the NLP subproblem for fixed y^k results, as only continuous variables are being considered.

$$\begin{aligned} \min_x \quad & C^k_{LB} = f(x, y^k) \\ \text{s.t.} \quad & g_j(x, y^k) \leq 0, \quad j \in \mathcal{J} \\ & x \in \mathcal{X} \end{aligned} \tag{P4}$$

If (P4) is infeasible the NLP feasibility subproblem for fixed y^k can be solved.

$$\begin{aligned} \min_x \quad & u \\ \text{s.t.} \quad & g_j(x, y^k) \leq u, \quad j \in \mathcal{J} \\ & x \in \mathcal{X}, \quad u \in \mathbb{R} \end{aligned} \tag{P5}$$

This NLP returns a strictly positive value for u.

Aside from the presented NLP's a linearized version of (P2) is regularly solved

$$\begin{aligned} \min_{x,y} \quad & C^k_L = \alpha \\ \text{s.t.} \quad & f(x^k, y^k) + \nabla f(x^k, y^k)^T \begin{bmatrix} x - x^k \\ y - y^k \end{bmatrix} \leq \alpha \\ & g_j(x^k, y^k) + \nabla g_j(x^k, y^k)^T \begin{bmatrix} x - x^k \\ y - y^k \end{bmatrix} \leq 0, \quad j \in \mathcal{J} \\ & x \in \mathcal{X}, \quad y \in \mathcal{Y}, \quad k = 1 \ldots K \end{aligned} \tag{P6}$$

The linearized problem can be constructed in several ways from the set of points K attained in previous iterations. Sometimes only violated or active constraints are linearized. When objective function and constraints are convex, the objective function is underestimated, while the constraints are overestimated. From the overestimated constraints stems the name outer approximation.

Branch & bound (B&B)

The branch and bound (B&B) algorithm has originally been proposed for linear problems, but has since been extended to handle non-linear objectives and constraints. As an initial step for the branch and bound the fully relaxed NLP (P3) is solved, which, as mentioned before, provides an absolute lower bound to the program in question. In the rare case that all relaxed integer variables assume integer values the optimal solution has been found and the algorithm can terminate. Otherwise a tree search is performed, exploring the space of the integer variables. In each step an increasing number of integer variables is fixed such that a NLP in the form of (P4) needs to be solved. The solution of these subproblems is a new lower bound for all descendant nodes. Further exploration of branches can be stopped, once a given subproblem returns a value grater than the current upper bound or becomes infeasible.

Due to the large number of NLP subproblems that have to be solved within the tree search, the branch and bound algorithm is most attractive, if the solution is computationally inexpensive, or few nodes have to be explored.

Outer approximation (OA)

The outer approximation (OA) algorithm relies on consecutively solving (P4) and (P6). Each solution of the NLP with fixed y^k yields a new point (x^k, y^k) which is used to construct an updated version of the MILP. The MILP generally includes linearized versions of all constraints and the objective function. As more and more points become available during the iterative process, new constraints are constructed for each available point.

The main theorem for the derivation of the OA algorithm states, that the optimal solution of the problem (P6) constructed from all points $(x^k, y^k), k \in K^*$. Where K^* is made up of all optimal solutions of (P4) where the current y^k yields a feasible solution, and (P5) where infeasible solutions of the NLP with fixed y^k are encountered. It should again be emphasized, that this theorem holds only for convex a objective function and constraints.

As the points necessary to construct the aforementioned system are not available when the solution process commences, a smaller systems is constructed and extended as more points become available. The first point again results from solving a fully relaxed system. This again yields an absolute lower bound for the original problem. The solution of each consecutive MILP gives a new lower bound which will always be greater than the bounds from previous iterations. Without any prove this argument is supported by the fact that adding new linear constraints will limit the feasible region of the problem and hence further restrict the possible solutions for the continuous variables.

is this true, that the fully relaxed system is initially solved??

The optimal points attained from the NLP subproblems with fixed discrete values form upper bounds on the optimal solution. Here no statement can be made about the quality of the bound in each step, but rather is the current upper bound updated, once a lower value is encountered.

The iterative process terminates, once the current upper and lower bound are within a given tolerance. It can be pointed out, that the outer approximation algorithm converges to the optimal solution in a single iteration if objective function and constraints in the original problem are linear, since in that case problems (P2) and (P6) are equivalent.

Generalized Benders decomposition (GBD)

The generalized Benders decomposition is very similar to the outer approximation algorithm. The main difference lies in way that (P6) is constructed. While for the outer approximation problem all constraints are included, in case of the GBD only active constraints are $J^k = \{j \mid g_j(x^k, y^k) = 0\}$ considered. Furthermore the set of continuous variables is eliminated by considering the KKT-conditions. The resulting problem

$$
\begin{aligned}
\min_{y} \quad & C_L^K = \alpha \\
\text{s.t.} \quad & f(x^k, y^k) + \nabla_y f(x^k, y^k)^T (y - y^k) \\
& \quad + (\mu^k)^T \left[g(x^k, y^k) + \nabla_y g(x^k, y^k)^T (y - y^k) \right] \leq \alpha, \quad k \in \mathcal{K}_{FS} \\
& (\lambda^k)^T \left[g(x^k, y^k) + \nabla_y g(x^k, y^k)^T (y - y^k) \right] \leq 0, \quad k \in \mathcal{K}_{IS}.
\end{aligned}
\tag{P7}
$$

Where $\mathcal{K}_{FS}$ and $\mathcal{K}_{IS}$ denote the sets of solutions for of feasible and infeasible iterations respectively.

This difference in formulation the MILP in the OA and GBD algorithm is what leads to the major computational differences. In general the MILP in the OA algorithm is expected to return tighter bounds than the respective problem in GBD. However the computational effort to solve the problem might be considerably higher for the OA case. Hence the GBD is expected to need more iterations, before converging, while the cost of a single iteration might be lower.

Extended cutting plane (ECP)

The extended cutting plane method requires no solution any NLP subproblems. Rather a version of the linearized problem is solved during each iteration. After each iteration the problem is extended by an addition cut or linearized constraint. Most commonly a linear version of the most violated constraint is added. A further possibility is to add all violated constraints to the problem. It should be noted, that for the ECP method the objective function has to be linear. If necessary non-linearities in the objective can be moved to the constraints by introduction of new variables.

LP/NLP branch & bound

5.2.2 Continuous reformulation

5.3 Optimization examples

The simulation of chemical processes supplies valuable insight into the

5.3.1 Degrees of freedom

In order to gain more insight into the behaviour of the dynamic models presented above an analysis of the degrees of freedom within the model is at hand. For the degrees of freedom the cost correlations will be disregarded, as they for a closed system of equations given the inputs generated form the column model. Furthermore interdependencies can be disregarded, as the cost model consist only of "forward" computations. In practical terms this statement can be confirmed since the models can be evaluated with and without costing equations. Hence only the stage and hydraulic equations will be considered.

For a given column without condenser or reboiler the model is made up of $[n_S(5n_C + 24) + n_F]$ differential algebraic equations in $[n_S(5n_C + 29) + n_F(n_S + n_C + 3) + 1]$ variables. In this isolated case all feed flow rates, their composition and enthalpies would be specified. In this case the feeds include a hypothetical condenser reflux (the upper most feed) as well as reboiler reflux (lowest feed). Along with the feeds and their qualities, the feed splits and reflux split have to be assigned. Lastly the column diameter needs to be known. This yields $[n_F(n_S + n_C + 2) + n_S + 1]$ specifications. To close the system initial conditions for all states have to be given. There are a total of $[4n_S]$ dynamic stages in a column section.

The condenser reboiler unit

5.3.2 Steady state single period

Objective function

$$CAPEX = \left(\sum_c C_c^{\text{cap}}\right) \cdot \left(q^{-a}\frac{q^a - 1}{q - 1}\right) + \sum_o C_o^{\text{oper}}$$
$$c = \{\text{HPC}, \text{LPC}, \text{CAC}, \text{HX}, \text{CP}, \text{CRM}, \text{CRCAC}\} \quad o = \{\text{CP}, \text{EXP}\} \quad (5.11)$$

Constraints : Limits on the product purities:

$$y_{1,N_2}^{HPC} \geq 0.985 \quad (5.12)$$
$$y_{1,N_2}^{LPC} \geq 0.985 \quad (5.13)$$
$$y_{1,Ar}^{CAC} \geq 0.985 \quad (5.14)$$
$$x_{reb}^{CRM} \geq 0.985 \quad (5.15)$$

No flooding in the columns:

$$d_{\text{column}}^{\text{HPC}} \geq d_{min}^{HPC} \quad (5.16)$$
$$d_{\text{column}}^{\text{LPC}} \geq d_{min}^{LPC} \quad (5.17)$$
$$d_{\text{column}}^{\text{CAC}} \geq d_{min}^{CAC} \quad (5.18)$$

No entrainment in the trayed column :

$$\left(1 - \sum_{k=1}^{j-1}\right) ent_k^{HPC} \leq 0.1 \quad (5.19)$$

Limit on cooling water outlet temperatures to prevent corrosion :

$$T_{\text{w,out}}^{IC1} \leq 323.15 \quad (5.20)$$
$$T_{\text{w,out}}^{IC2} \leq 323.15 \quad (5.21)$$
$$T_{\text{w,out}}^{IC3} \leq 323.15 \quad (5.22)$$

Design Variables

- HPC diameter $d_{\text{column}}^{\text{HPC}}$
- LPC diameter $d_{\text{column}}^{\text{LPC}}$
- CAC diameter $d_{\text{column}}^{\text{CAC}}$
- HPC reflux location ζ_{HPC}^{R}
- LPC reflux location ζ_{LPC}^{R}
- CAC reflux location ζ_{CAC}^{R}
- LPC CAC side draw location $\zeta_{2,j}^{SV,\text{LPC}}$
- heat exchange area multi-stream heat exchanger $A_{\text{HX}}^{multiHX}$
- heat exchange area main condenser reboiler A_{HX}^{CRM}
- heat exchange area CAC condenser reboiler A_{HX}^{CRCAC}

Manipulated Variables

- intercooler outlet temperatures ($T_{\text{out}}^{IC1}, T_{\text{out}}^{IC2}, T_{\text{out}}^{IC3}$)
- HPC dimensionless side draw (gaseous N_2product) ($s_1^{V,\text{HPC}}$)
- LPC dimensionless side draws ($s_i^{V,\text{LPC}}$)

5.3.3 Optimization & control

To include the design of a PI control structure in the process, the following constraints need to be added.

$$u_m = b_{m,1} + \sum_{j=1}^{n_m} \left(K_{m,n} \cdot e_{m,n} + I_{m,n}\right), \qquad m = 1 \dots n_{in}, \tag{5.23}$$

$$e_{m,n} = set_{m,n} - meas_n \qquad m = 1 \dots n_{in}, n = 1 \dots n_m, \tag{5.24}$$

$$\frac{\mathrm{d}I}{\mathrm{d}t} = \frac{e_{m,n}}{\tau_{m.n}} \qquad m = 1 \dots n_{in}, n = 1 \dots n_m, \tag{5.25}$$

$$\frac{\mathrm{d}I}{\mathrm{d}t} = 0 \qquad m = 1 \dots n_{in}, n = 1 \dots n_m, \tag{5.26}$$

$$set_{m,n} = set_{m-1,n} \qquad m = 2 \dots n_{in}, n = 1 \dots n_m, \tag{5.27}$$

$$K_{m,n}^{L} \cdot \zeta_{m,n}^{C} \leq K_{m,n} \leq K_{m,n}^{U} \qquad m = 1 \dots n_{in}, n = 1 \dots n_m, \tag{5.28}$$

$$\sum_{m=1}^{n_m} \zeta_{m,n}^{C} = 1 \qquad m = 1 \dots n_{in}, \tag{5.29}$$

$$\sum_{n=1}^{n_{in}} \zeta_{m,n}^{C} = 1 \qquad n = 1 \dots n_m, \tag{5.30}$$

Since new states have been introduced, the corresponding initial conditions will have to be included

$$I_{m,n}(t = 0) = 0, \qquad m = 1 \ldots n_{in}, n = 1 \ldots n_m \tag{5.31}$$

$$e_{m,n}(t = 0) = 0, \qquad m = 1 \ldots n_{in}, n = 1 \ldots n_m \tag{5.32}$$

$$\tag{5.33}$$

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Todo list