CHE656 Design Projects

Semester 2, 2021, Part (b)

Problem Statement

Using Metaheuristic Algorithms to Solve Complex
Chemical Engineering Optimization Problems

Adapted from http://www.scholarpedia.org/article/Metaheuristic_Optimization

Introduction

Most real-world optimizations are highly nonlinear, multimodal, and under various complex constraints. Similarly, many optimization problems found in chemical engineering are very complex and combinatorial in nature. The complexity in these problems arise mainly from two inherent factors: (1) the solution space of these problems increases exponentially as the problem size increases (hence, the word "combinatorial", and (2) Many local optima exist and so even when a good or optimal solution is found, there is no guarantee and no way of knowing if that solution is a global optimum.

Examples of combinatorial optimization problems in chemical engineering are:

- Product scheduling of batch processes
- Optimization of metabolic pathways and diversification of protein coding sequences and many other bioengineering problems.
- Optimization problems involving multi-objective functions
- Synthesis of heat exchanger networks
- MILP and MINLP problems in chemical engineering, such as design of batch processes

Metaheuristic optimization algorithms are one class of optimization techniques that espouses a "master strategy that guides and modifies other heuristics to produce solutions beyond those that are normally generated in a quest for local optimality" (Glover and Laguna 1997). These algorithms are often inspired by the working of nature and have been shown to be able to locate global optimum more often than simple heuristics or conventional optimization techniques.

Some of the traditional and well-known metaheuristic optimization algorithms are:

1. Simulated Annealing (SA)
2. Genetic Algorithms (GA)
3. Ant Colony Optimization (ACO)
4. Bee Algorithms (BA)
5. Particle Swarm Optimization (PSO)
6. Tabu Search (TS)

For a quick introduction to metaheuristic optimization and brief descriptions of each algorithm, see the following link: http://www.scholarpedia.org/article/Metaheuristic_Optimization.

New optimization metaheuristics are continually being developed. In recent years, there have been a flurry of activities in this field, because as mentioned above, optimization problems arise in many disciplines, and not just in chemical engineering. Below is a list of metaheuristics collected from https://en.wikipedia.org/wiki/Talk:Metaheuristic/List_of_Metaheuristics.

- 1952: Robbins and Monro work on stochastic optimization methods.
- 1952: Fermi and Metropolis develop an early form of pattern search as described belatedly by Davidon.
- 1954: Barricelli carry out the first simulations of the evolution process and use them on general optimization problems.
- 1963: Rastrigin proposes random search.
- 1965: Matyas proposes random optimization.
- 1965: Rechenberg proposes evolution strategy.
- 1965: Nelder and Mead propose a simplex heuristic, which was shown by Powell to converge to non-stationary points on some problems.
- 1966: Fogel et al. propose evolutionary programming.
- 1970: Hastings proposes the Metropolis-Hastings algorithm.
- 1970: Cavicchio proposes adaptation of control parameters for an optimizer.
- 1970: Kernighan and Lin propose a graph partitioning method, related to variable-depth search and prohibition-based (tabu) search
- 1975: Holland proposes the genetic algorithm.
- 1977: Glover proposes Scatter Search.
- 1978: Mercer and Sampson propose a metaplan for tuning an optimizer's parameters by using another optimizer.
- 1980: Smith describes genetic programming.

- 1983: Kirkpatrick et al. propose simulated annealing.
- 1986: Glover proposes tabu search, first mention of the term *metaheuristic*.
- 1986: Farmer et al. work on the artificial immune system.
- 1986: Grefenstette proposes another early form of metaplan for tuning an optimizer's parameters by using another optimizer.
- 1988: First conference on genetic algorithms is organized at the University of Illinois at Urbana-Champaign.
- 1988: Koza registers his first patent on genetic programming.
- 1989: Goldberg publishes a well known book on genetic algorithms.
- 1989: Evolver, the first optimization software using the genetic algorithm.
- 1989: Moscato proposes the memetic algorithm.
- 1991: Interactive evolutionary computation.
- 1992: Dorigo proposes the ant colony algorithm.
- 1993: The journal, *Evolutionary Computation*, begins publication by the Massachusetts Institute of Technology.
- 1993: Fonseca and Fleming propose MOGA for multiobjective optimization.
- 1994: Battiti and Tecchiolli propose Reactive Search Optimization(RSO) principles for the online self-tuning of heuristics.
- 1994: Srinivas and Deb propose NSGA for multiobjective optimization.
- 1995: Kennedy and Eberhart propose particle swarm optimization.
- 1995: Wolpert and Macready prove the no free lunch theorems.
- 1996: Mühlenbein and Paaß work on the estimation of distribution algorithm.
- 1996: Hansen and Ostermeier propose CMA-ES.
- 1997: Storn and Price propose differential evolution.
- 1997: Rubinstein proposes the cross entropy method.
- 1999: Taillard and Voss propose POPMUSIC.
- 2001: Geem et al. propose harmony search.
- 2001: Hanseth and Aanestad introduce the Bootstrap Algorithm.
- 2002: Deb et al. propose NSGA-II for multiobjective optimization.
- 2004: Nakrani and Tovey propose bees optimization.
- 2005: Krishnanand and Ghose propose Glowworm swarm optimization.
- 2005: Karaboga proposes Artificial Bee Colony Algorithm (ABC).
- 2005: Duc-Truong Pham et al. proposed Bees Algorithms (BA)
- 2006: Haddad et al. introduces honey-bee mating optimization.
- 2007: Hamed Shah-Hosseini introduces Intelligent Water Drops.
- 2007: Atashpaz-Gargari introduces Imperialist competitive algorithm.

- 2008: Wierstra et al. propose natural evolution strategies based on the natural gradient.
- 2008: Yang introduces firefly algorithm.
- 2008: Mucherino and Seref propose the Monkey Search
- 2009: Ali Husseinzadeh Kashan introduced the League Championship Algorithm (LCA).
- 2009: Kadioglu and Sellmann introduce Hegel and Fichte's dialectic as a local search meta-heuristic Dialectic Search.
- 2009: Yang and Deb introduce cuckoo search.
- 2009: Rashedi proposes Gravitational Search Algorithm
- 2009: Josue Cuevas et al. propose Virus Optimization Algorithm
- 2010: Yang develops bat algorithm.
- 2011: Hamed Shah-Hosseini proposes the Galaxy-based Search Algorithm.
- 2011: Tamura and Yasuda propose spiral optimization.
- 2012: Civicioglu proposes Differential Search Algorithm. Matlab code-link has been provided in Çivicioglu, P.,(2012). and Matlab File Exchange.
- 2013: Civicioglu proposes Artificial Cooperative Search Algorithm (ACS).
- 2015: Election Algorithm: A new socio-politically inspired strategy — Preceding unsigned comment added by 2.187.47.244 (talk) 07:31, 23 June 2016 (UTC)

However, it has been argued that many of these optimization metaheuristic algorithms are very similar and are variations of the same theme. Moreover, many of these proposed metaheuristics have never been applied in the real world, so their effectiveness has yet to be validated. A recent article titled "Nature Inspired Optimization Algorithms or Simply Variations of Metaheuristics?" (Tzanetos A and Dounias G., August 2020) and published in *Artificial Intelligence Review* gives a very comprehensive review on the current status of nature-inspired optimization algorithms proposed in the past decade.

Your Assignment

Your design problem Part (b) assignments for this semester (CHE656) will involve the following tasks:

1. Each team will be assigned a metaheuristic optimization algorithm.

2. Study references and papers that were given to you by the course instructor your assigned metaheuristic.

3. Search the Internet and find more relevant papers on your assigned metaheuristic and read them carefully.

4. Finally, code the metaheuristics you have been assigned in MATLAB and assess its effectiveness in terms of accuracy and required computation time using optimization benchmark problems, including some chemical engineering problems, provided in this handout. You are not allowed to use off-the-shelf software or functionalities such as the Global Search Toolbox in MATLAB to solve problems. However, you may compare the solutions from your coding with those found by the software.

Again, you must test your metaheuristic optimization algorithm on the benchmark problems given in this document. The benchmark problems are divided into two categories. The first category consists of generic or general optimization problems, while the second category consists of optimization problems in chemical engineering. Note that optimal solutions or best solutions reported are given for some problems but not others in this document. During the course of Semester 2, the course instructor will provide you with more solutions. After that, you are at the liberty to choose a few chemical engineering problems to solve. The only requirement is that these chemical engineering problems should be sufficiently complex that the optimum solutions are hard to obtain and that conventional optimization techniques fail to give satisfactory answers. Note that you may need to consult optimization textbooks and published papers to find suitable optimization problems in chemical engineering.

Finally, a large library of optimization test problems in mathematical formulations can be found at this link: http://www.sfu.ca/~ssurjano/optimization.html.

Note that some of the metaheuristic algorithms were designed to solve both unconstrained and constrained optimization problems. However, most of them were not designed to solve optimization problems involving discrete or integer variables. Hence, you will need to be creative and find ways to modify a given metaheuristic so it can be used to solve all types of test problems given, including scheduling problems. For example, you can incorporate the Penalty Method to convert a constrained problem into an unconstrained one.

Benchmark Problem #1

The design of a compressional and tensional spring involves three design variables: wire diameter x_1, coil diameter x_2, and the length of the coil x_3. This optimization can be written as:

$$\text{minimize} \;\; f(\mathbf{x}) = x_1^2 x_2 (2 + x_3),$$

$$g_1(\mathbf{x}) = 1 - \frac{x_2^3 x_3}{71785 x_1^4} \leq 0,$$

$$g_2(\mathbf{x}) = \frac{4x_2^2 - x_1 x_2}{12566(x_1^3 x_2 - x_1^4)} + \frac{1}{5108 x_1^2} - 1 \leq 0,$$

$$g_3(\mathbf{x}) = 1 - \frac{140.45 x_1}{x_2^3 x_3} \leq 0,$$

$$g_4(\mathbf{x}) = \frac{x_1 + x_2}{1.5} - 1 \leq 0.$$

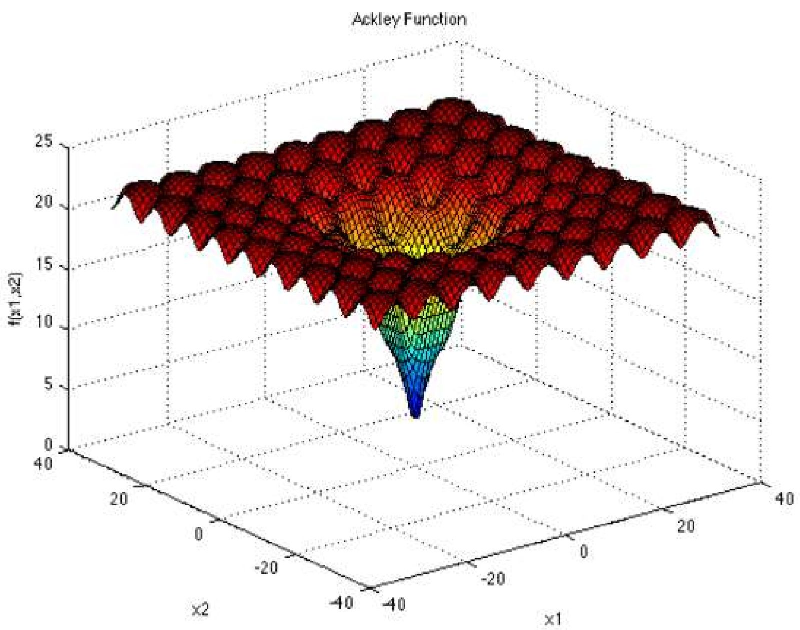
$$0.05 \leq x_1 \leq 2.0, \quad 0.25 \leq x_2 \leq 1.3, \quad 2.0 \leq x_3 \leq 15.0.$$

The best solution for this problem is $\boldsymbol{x}^*$ = [0.051690, 0.356750, 11.28126] with $f(\boldsymbol{x}^*)$ =0.012665.

Benchmark Problem #2

The Ackley function is widely used for testing optimization algorithms. In its two-dimensional form, as shown in the plot above, it is characterized by a nearly flat outer region, and a large hole at the center. The function poses a risk for optimization algorithms, particularly hill-climbing algorithms, to be trapped in one of its many local minima.

Recommended variable values are: $a = 20$, $b = 0.2$ and $c = 2\pi$.



$$f(\mathbf{x}) = -a \exp\left(-b\sqrt{\frac{1}{d}\sum_{i=1}^{d} x_i^2}\right) - \exp\left(\frac{1}{d}\sum_{i=1}^{d}\cos(cx_i)\right) + a + \exp(1)$$

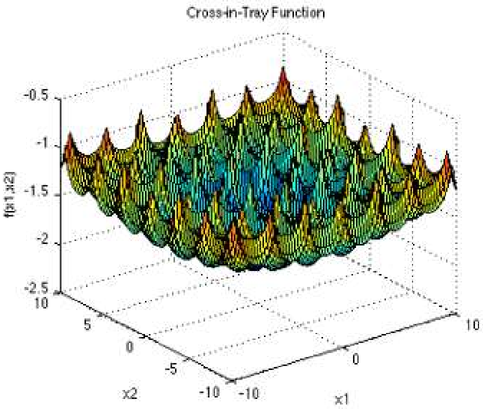
Solve this optimization problem when:

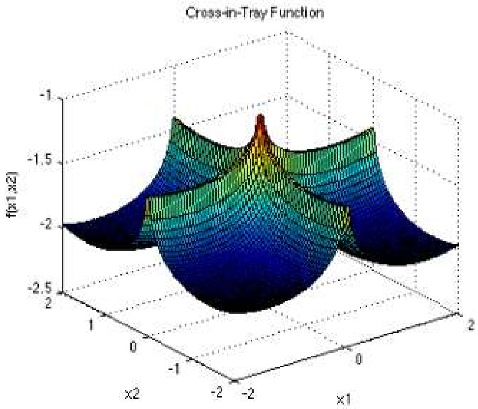
1. $d = 2$ (two-dimensional). The global minimum is $\boldsymbol{x}^* = [0, 0]$ with $f(\boldsymbol{x}^*) = 0$

2. $d = 5$

Benchmark Problem #3

The Cross-in-Tray function has multiple global minima. It is shown here with a smaller domain in the second plot, so that its characteristic "cross" will be visible.





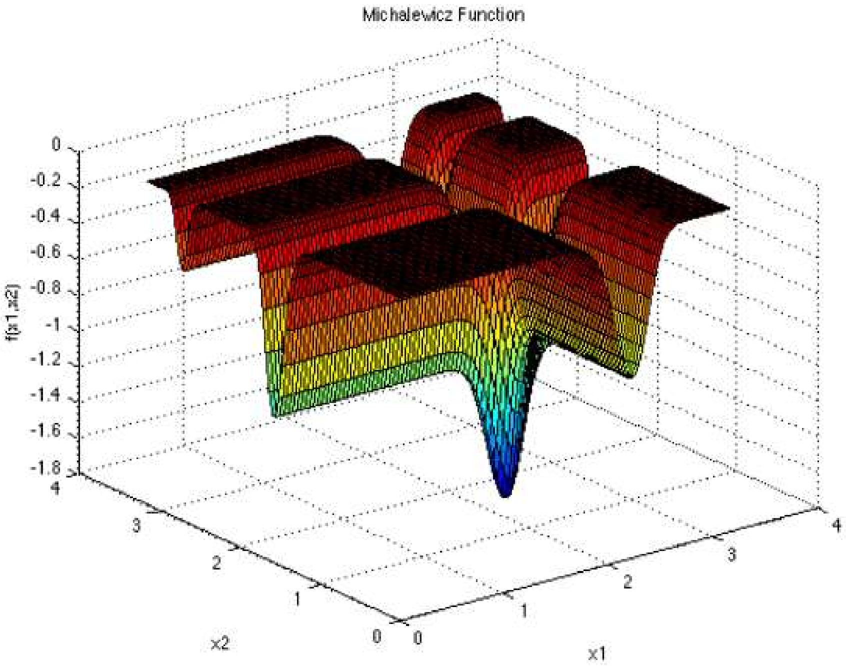
$$f(\mathbf{x}) = -0.0001\left(\left|\sin(x_1)\sin(x_2)\exp\left(\left|100 - \frac{\sqrt{x_1^2+x_2^2}}{\pi}\right|\right)\right|+1\right)^{0.1}$$

Global Minima:

$f(\mathbf{x}^*) = -2.06261$, at $\mathbf{x}^* = (1.3491, -1.3491), (1.3491, 1.3491), (-1.3491, 1.3491)$ and $(-1.3491, -1.3491)$

Benchmark Problem #4

The Michalewicz function has d! local minima, and it is multimodal. The parameter m defines the steepness of these valleys and ridges; a larger m leads to a more difficult search. The recommended value of m is m = 10. The function's two-dimensional form is shown in the plot above.



$$f(\mathbf{x}) = -\sum_{i=1}^{d} \sin(x_i)\sin^{2m}\left(\frac{ix_i^2}{\pi}\right)$$

Solve this optimization problem when d = 2, 5, and 10 (with m = 10).

Global Minima:

at $d = 2$: $f(\mathbf{x}^*) = -1.8013$, at $\mathbf{x}^* = (2.20, 1.57)$
at $d = 5$: $f(\mathbf{x}^*) = -4.687658$
at $d = 10$: $f(\mathbf{x}^*) = -9.66015$

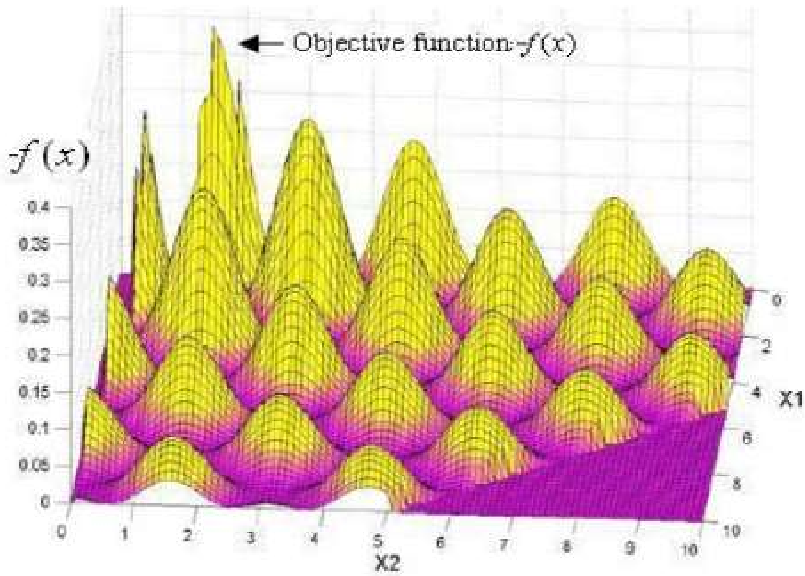
Benchmark Problem #5

The following optimization problem is known as Keane's "bump" function (Andy Keane, 1994) which seeks to minimize a very complex objective function with constraints as follows:

$$Minimize\ f(x) = -\left| \left\{ \sum_{i=1}^{m} \cos^4(x_i) - 2\prod_{i=1}^{m} \cos^2(x_i) \right\} \Big/ \left(\sum_{i=1}^{m} i x_i^2 \right)^{0.5} \right|$$

$$\text{subject to: } g_1(x):\ 0.75 - \prod_{i=1}^{m} x_i < 0; \quad g_2(x):\ \sum_{i=1}^{m} x_i - 7.5m < 0; \quad 0 < x_i < 10.$$

Fig.-1: Keane's Bump Function in 2 Dimensions



Source: Hacker, Eddy and Lewis (2002)

A visual appreciation of Keane's two-dimensional (m=2) bump function may be obtained from the graphical presentation (Fig.-1; Hacker et al., 2002).

As the dimension (m) grows larger, the optimum value of the function becomes more and more difficult to obtain.

Keane (1994) observed that for m=20 the value of min[f(x)] could be about -0.76 and for m=50 it could be about -0.835 but did not know this to be the case.

Solve this problem when m = 2, 5, and 20, i.e. there is a total of three separate objective functions to minimize.

Benchmark Problem #6

The three-bar truss design problem (Askarzadeh A. 2016) is about minimization of the volume of a statistically loaded three-bar truss subject to stress (σ) constraints on each of the truss members by adjusting cross sectional areas (x_1 and x_2). This optimization problem consists of two continuous decision variables and three nonlinear inequality constraints as follows:

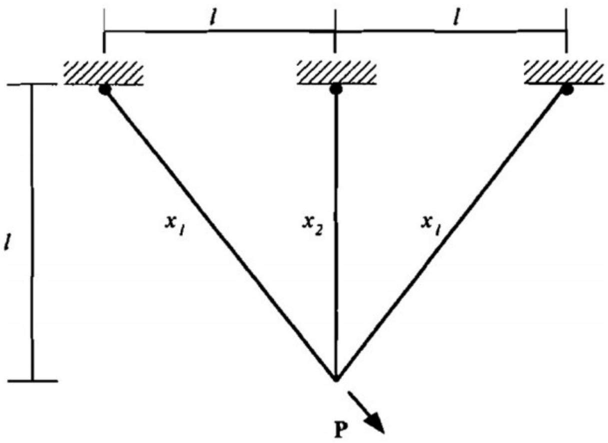
Minimization: $f(x) = (2\sqrt{2}x_1 + x_2) \times l$

Subject to $g_1(x) = \frac{\sqrt{2}x_1 + x_2}{\sqrt{2}x_1^2 + 2x_1x_2} P - \sigma \leq 0$

$$g_2(x) = \frac{x_2}{\sqrt{2}x_1^2 + 2x_1x_2} P - \sigma \leq 0$$

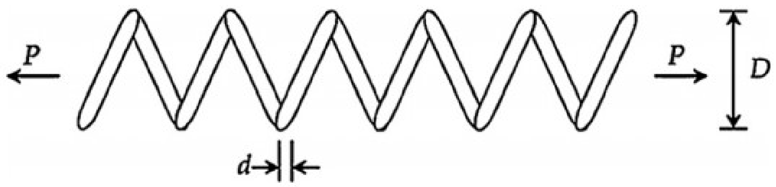
$$g_3(x) = \frac{1}{\sqrt{2}x_2 + x_1} P - \sigma \leq 0$$

The problem is usually evaluated on $x_i \in [0,1]$ for $i = 1, 2$. In addition, the *l, P* and σ constants are 100 cm, 2 kN/cm^2 and 2 kN/cm^2, respectively. The figure below shows a schematic of three-bar truss design problem.



Benchmark Problem #7

The tension/compression spring design problem (Askarzadeh A. 2016) as shown in the figure below is about the minimization of the weight of a tension/compression spring.



There are three continuous decision variables, namely the wire diameter (d or x_1), the mean coil diameter (D or x_2), and the number of active coils (P or x_3). This problem has one linear and three nonlinear inequality constraints.

Minimization: $f(x) = x_1^2 x_2 (2 + x_3)$

Subject to

$$g_1(x) = 1 - \frac{x_2^3 x_3}{71785 x_1^4} \le 0$$

$$g_2(x) = \frac{4x_2^2 - x_1 x_2}{12566(x_1^3 x_2 - x_1^4)} + \frac{1}{5108 x_1^2} - 1 \le 0$$

$$g_3(x) = 1 - \frac{140.45 x_1}{x_2^3 x_3} \le 0$$

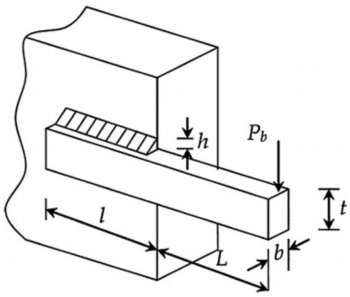
$$g_4(x) = \frac{x_1 + x_2}{1.5} - 1 \le 0$$

Domain:

$$0.05 \le x_1 \le 2.0$$
$$0.25 \le x_2 \le 1.3$$
$$2.0 \le x_3 \le 15.0$$

Benchmark Problem #8

The welded beam design problem (Askarzadeh A. 2016) is about the minimization of the cost of a welded beam. There are four continuous design variables with two linear and five nonlinear inequality constraints based on shear stress (τ), bending stress in the beam (σ), bucking load on the bar (P_b), end deflection of the beam (δ), and side constraints. The figure below shows a schematic of welded beam design problem. The decision variables are x_1 or h, x_2 or l, x_3 or t, and x_4 or b.



Minimization: $f(x) = 1.10471x_1^2x_2 + 0.04811x_3x_4(14 + x_2)$

Subject to

$$g_1(x) = \tau(x) - \tau_{max} \leq 0$$

$$g_2(x) = \sigma(x) - \sigma_{max} \leq 0$$

$$g_3(x) = x_1 - x_4 \leq 0$$

$$g_4(x) = 0.10471x_1^2 + 0.04811x_3x_4(14 + x_2) - 5 \leq 0$$

$$g_5(x) = 0.125 - x_1 \leq 0$$

$$g_6(x) = \delta(x) - \delta_{max} \leq 0$$

$$g_7(x) = P - P_c(x) \leq 0$$

where

$$\tau(x) = \sqrt{(\tau')^2 + 2\tau'\tau''\frac{x_2}{2R} + (\tau'')^2}$$

$$\tau' = \frac{P}{\sqrt{2}x_1x_2}, \quad \tau'' = \frac{MR}{J}, \quad M = P\left(L + \frac{x_2}{2}\right)$$

$$R = \sqrt{\frac{x_2^2}{4} + \left(\frac{x_1 + x_3}{2}\right)^2}, \quad \delta(x) = \frac{4PL^3}{Ex_3^3x_4}$$

$$J = 2\left[\sqrt{2}x_1x_2\left\{\frac{x_2^2}{12} + \left(\frac{x_1 + x_3}{2}\right)^2\right\}\right], \quad \sigma(x) = \frac{6PL}{x_4x_3^2}$$

$$P_c(x) = \frac{4.013E\sqrt{\frac{x_3^2x_4^6}{36}}}{L^2}\left(1 - \frac{x_3}{2L}\sqrt{\frac{E}{4G}}\right)$$

$$P = 6000 \text{ lb}, L = 14 \text{ in}, \quad E = 30e6 \text{ psi}$$

$$G = 12e6 \text{ psi}, \tau_{\max} = 13,600 \text{ psi}, \sigma_{\max} = 30,000 \text{ psi}$$

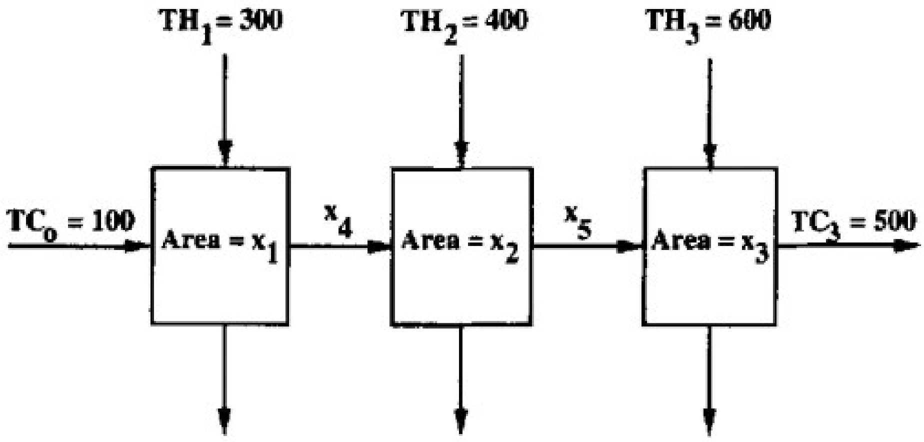
$$\delta_{\max} = 0.25 \text{ in}, \quad 0.1 \leqslant x_1 \leqslant 2, 0.1 \leqslant x_2 \leqslant 10$$

$$0.1 \leqslant x_3 \leqslant 10, 0.1 \leqslant x_4 \leqslant 2$$

Chemical Engineering Benchmark Problems

ChE Problem #1:

This problem is a heat exchanger network design. The objective is to find the minimum area of three heat exchangers as shown in the figure below. They are responsible for heating a cold stream whose heat capacity flow rate is 100,000 kW/°F from 100 to 500°F. The overall coefficient of Heatex1, Heatex2 and Heatex3 are 120, 80 and 40 kW/ft^2°F, respectively.



This problem can be formulated as follows:

Minimization: $x_1 + x_2 + x_3$

Subject to $100000(x_4 - 100) = 120x_1(300 - x_4)$

$100000(x_5 - x_4) = 80x_2(400 - x_5)$

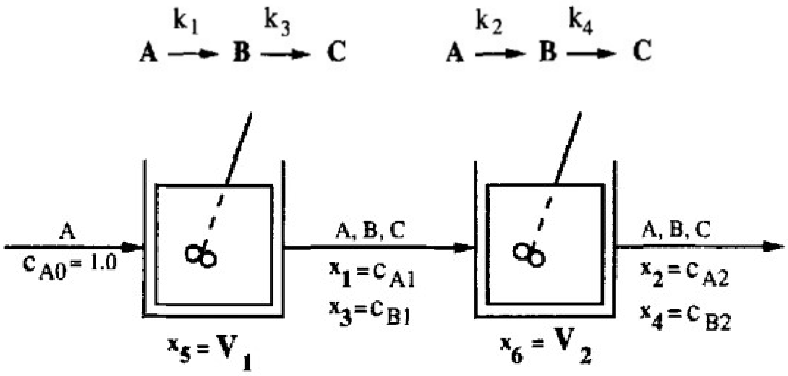
$100000(500 - x_5) = 40x_3(600 - 500)$

$(0, 0, 0, 100, 100) \leq \boldsymbol{x} \leq (15834, 36250, 10000, 300, 400)$

The global optimum is $\boldsymbol{x}^* = (579.306743, 1359.971266, 5109.971263, 182.017600, 295.601150)$ with $f(\boldsymbol{x}^*) = 7049.249$.

ChE Problem #2:

This is a reactor sequence design with capital cost constraints. Considering the reaction sequence A→B→C and assuming first order kinetics for both reactions, design a sequence of two reactors such that the concentration of *B* in the exit stream of the second reactor (C_{B2}) is maximized and the investment cost does not exceed a given upper bound.



where $k_1 = 0.09755988\ s^{-1}$, $k_2 = 0.99k_1\ s^{-1}$, $k_3 = 0.0391908\ s^{-1}$ and $k_4 = 0.9k_3\ s^{-1}$. Let V_1, V_2 be the residence times for the first and second reactor respectively. Then, the reactor design problem is formulated as a nonlinear programming problem:

Maximization: x_4

Subject to $(x_1 - 1) + k_1 x_1 x_5 = 0$

$(x_2 - x_1) + k_2 x_2 x_6 = 0$

$(x_3 + x_1 - 1) + k_3 x_3 x_5 = 0$

$(x_4 - x_3 + x_2 - x_1) + k_4 x_4 x_6 = 0$

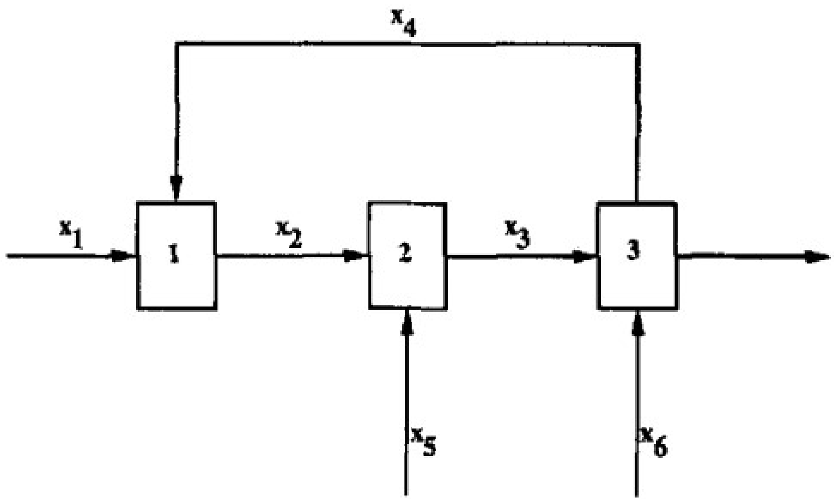
$x_5^{0.5} + x_6^{0.5} \leq 4$

$0 \leq \boldsymbol{x} \leq (1, 1, 1, 1, 16, 16)$

The first four constraints involve the reaction kinetics of all reactions in both reactors. Assuming that the capital cost of a reactor is proportional to the square root of its residence time, this capital cost constraint is the fifth constraint. The global optimum is at $\boldsymbol{x}^*$ = (0.771462, 0.516997, 0.204234, 0.388812, 3.036504, 5.096052) with $f(\boldsymbol{x}^*) = 0.388812$.

ChE Problem #3:

This is the design of a three-stage process system with recycle which was improved by Stephanopoulos and Westerberg from two-stages example taken from McGalliard's thesis.



Minimization: $x_1^{0.6} + x_2^{0.6} + x_3^{0.4} - 4x_3 + 2x_4 + 5x_5 - x_6$

Subject to $-3x_1 + x_2 - 3x_4 = 0$

$-2x_2 + x_3 - 2x_5 = 0$

$4x_4 - x_6 = 0$

$x_1 + 2x_4 \le 4$

$x_2 + x_5 \le 4$

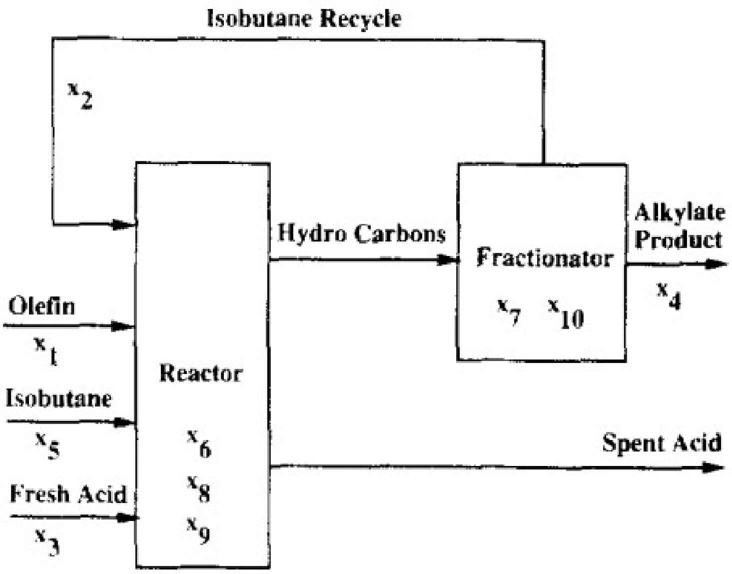
$x_3 + x_6 \le 6$

$0 \le \boldsymbol{x} \le (3, 4, 4, 2, 2, 6)$

The global optimum is at $\boldsymbol{x}^* = (0.166667, 2, 4, 0.5, 0, 2)$ with $f(x^*) = -13.401904$.

ChE Problem #4:

This problem is called "Alkylation Process Optimization". The original was proposed by Bracken and McCoarmick, and modified by Liebman, Quesada and Grossmann. It is a model for optimization of the operation of a chemical process common in the petroleum industry. The model seeks to determine the optimum set of operating conditions for the process, a profit function to be maximized and a set of starting conditions. It is a fairly large problem.



Minimization: $5.04x_1 + 0.035x_2 + 10x_3 + 3.36x_5 - 0.063x_4x_7$

Subject to $x_1 = 1.22x_4 - x_5$

$x_9 + 0.222x_{10} = 35.82$

$3x_7 - x_{10} = 133$

$x_7 = 86.35 + 1.098x_8 - 0.038x_8^2 + 0.325(x_6 - 89)$

$x_4x_9 + 1000x_3 = 98000x_3/x_6$

$x_2 + x_5 = x_1x_8$

$1.12 + 0.13167x_8 - 0.00667x_8^2 \geq x_4/x_8$

$(1, 1, 0, 1, 85, 90, 3, 1.2, 145) \leq \boldsymbol{x} \leq (2000, 16000, 120, 5000, 2000, 93, 95, 12, 4, 162)$

The global optimum is at $\boldsymbol{x}^*$ = (1728.310416, 16000, 98.133457, 3055.992144, 2000, 90.618812, 94.189777, 10.414796, 2.615609, 149.569330) with $f(\boldsymbol{x}^*) = -1161.336694$.