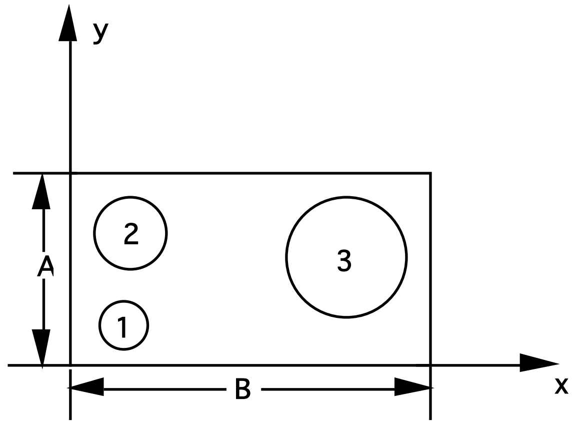
06-606 **Computational Methods** **Fall, 2016**
Due: 11/29/16

1. Consider the nonconvex, constrained NLP:



Min $(A + B)$

$$\begin{cases} x_1,\ y_1 \ge R_1 & x_1 \le B - R_1,\ y_1 \le A - R_1 \\ x_2,\ y_2 \ge R_2 & x_2 \le B - R_2,\ y_2 \le A - R_2 \\ x_3,\ y_3 \ge R_3 & x_3 \le B - R_3,\ y_3 \le A - R_3 \end{cases}$$

$$\text{no overlaps} \begin{cases} (x_1 - x_2)^2 + (y_1 - y_2)^2 \ge (R_1 + R_2)^2 \\ (x_1 - x_3)^2 + (y_1 - y_3)^2 \ge (R_1 + R_3)^2 \\ (x_2 - x_3)^2 + (y_2 - y_3)^2 \ge (R_2 + R_3)^2 \end{cases}$$

$$x_1, x_2, x_3, y_1, y_2, y_3,\ A, B \ge 0$$

Write the Kuhn Tucker conditions for this problem.

a) Show that this problem is nonconvex

b) What can you say about the optimal active set of inequalities for this problem?

c) How does the system of Kuhn Tucker conditions lead to multiple NLP solutions?

2. Consider the NLP:

$$\begin{aligned} &\text{Min } x_2 \\ \text{s.t.} \quad & x_1 - x_2^2 + 1 \le 0 \\ & -x_1 - x_2^2 + 1 \le 0 \end{aligned}$$

a) Sketch the feasible region for this problem

b) Using GAMS, what happens if $x_1 = x_2 = 0$ is chosen as a starting point and SQP (SNOPT) or reduced gradient methods (CONOPT) are applied?

3. While searching for the minimum of

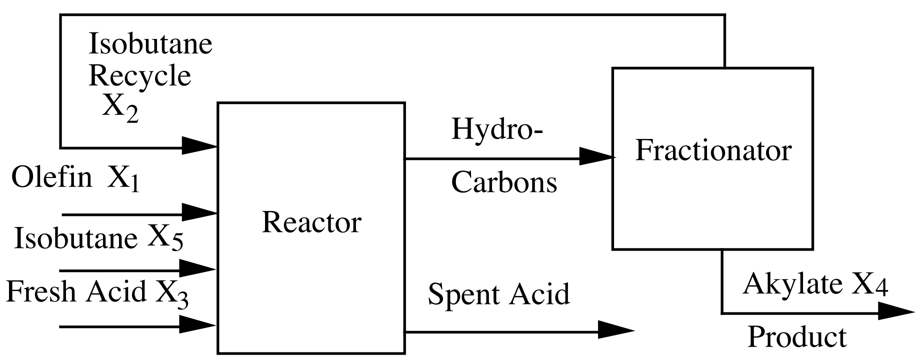
$$f(x) = [x_1^2 + (x_2 + 1)^2][x_1^2 + (x_2 - 1)^2]$$

we terminate the following points

a) $x^{(1)} = [0,0]^T$
b) $x^{(2)} = [0,1]^T$
c) $x^{(3)} = [0,-1]^T$
d) $x^{(4)} = [1,1]^T$

Classify each point.

4. See the Brief Tutorial on GAMS and download GAMS from www.gams.com. Consider the alkylation process shown below from Bracken & McCormick (1968)



X_1 = Olefin feed (barrels per day)
X_2 = Isobutane recycle (barrels per day)
X_3 = Acid addition rate (1000s pounds/day)
X_4 = Alkylate yield (barrels/day)
X_5 = Isobutane input (barrels per day)
X_6 = Acid strength (weight percent)
X_7 = Motor octane number alkylate
X_8 = External isobutane-to-olefin ratio
X_9 = Acid dilution factor
X_{10} = F-4 performance no. of alkylate

The alkylation is derived from simple mass balance relationships and regression equations determined from operating data. The first four relationships represent characteristics of the alkylation reactor and are given empirically.

The alkylate field yield, X4, is a function of both the olefin feed, X1, and the external isobutane to olefin ratio, X8. The following relation is developed from a nonlinear regression for temperature between 80 and 90 degrees F and acid strength between 85 and 93 weight percent:

X4 = X1*(1.12 + .12167*X8 - 0.0067*X8**2)

The motor octane number of the alkylate, X7, is a function of X8 and the acid strength, X6. The nonlinear regression under the same conditions as for X4 yields:

X7 = 86.35 + 1.098*X8 - 0.038*X8**2 + 0.325*(X6-89.)

The acid dilution factor, X9, can be expressed as a linear function of the F-4 performance number, X10 and is given by:

X9 = 35.82 - 0.222*X10

Also, X10 is expressed as a linear function of the motor octane number, X7.

X10 = 3*X7 - 133

The remaining three constrants represent exact definitions for the remaining variables. The external isobutane to olefin ratio is given by:

X8 = (X2 + X5)/X1

To prevent potential zero divides it is rewritten as:

X8*X1 = X2 + X5

The isobutane feed, X5, is determined by a volume balance on the system. Here olefins are related to alkylated product and there is a constant 22% volume shrinkage, thus giving X4 = X1 + X5 - 0.22*X4 or:

X5 = 1.22*X4 - X1

Finally, the acid dilution strength (X6) is related to the acid addition rate (X3), the acid dilution factor (X9) and the alkylate yield (X4) by the equation, 1000*X3 + X4*X6*X9(98 - X6). Again, we reformulate this equation to eliminate the division and obtain:

X6*(Xr*X9+1000*X3) = 98000*X3

The objective function is a straightforward profit calculation based on the following data:

- Alkylate product value = \$0.063/octane-barrel
- Olefin feed cost = \$5.04/barrel
- Isobutane feed cost = \$3.36/barrel
- Isobutane recycle cost = \$0.035/barrel
- Acid addition cost = \$10.00/barrel

This yields the objective function to be maximized is therefore the profit (\$/day)

OBJ = 0.063*X4*X7 - 5.04*X1 - 0.035*X2 - 10*X3 - 3.36*X5

The following exercises are based on the description in Liebman et al (1984).

a) Set up this NLP problem and solve.

b) The regression equations presented in section 2 are based on operating data and are only approximations and it is assumed that equally accurate expressions actually lie in a band around these expressions. Therefore, in order to consider the effect of this band, Liebman et al (1984) suggested a relaxation of the regression variables. Replace the variables X4, X7, X9 and X10 with RX4, RX7, RX9 and RX10 in the regression equations (only) and impose the constraints:

$$0.99*X4 \le RX4 \le 1.01*X4$$
$$0.99*X7 \le RX7 \le 1.01*X7$$
$$0.99*X9 \le RX9 \le 1.01*X9$$
$$0.9*X10 \le RX10 \le 1.11*X10$$

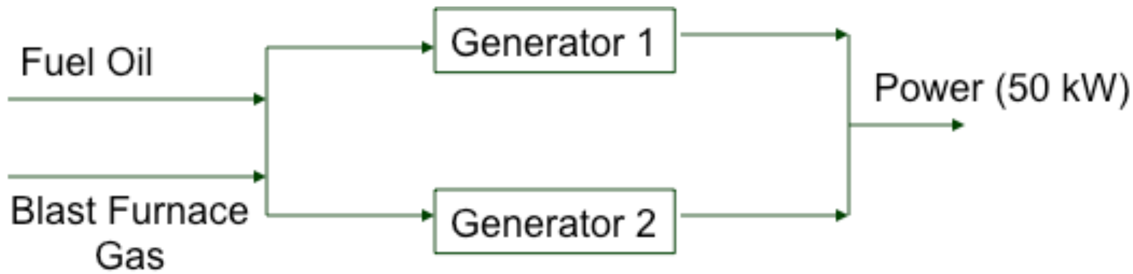
to allow for the relaxation. Resolve with this formulation. How would you interpret these results?

4. Power generation from Fuel Oil (CAChE Case Study by Prof. I. A. Karimi, NUS, file: fueloil.gms)

A two-boiler turbine-generator combination below is used to produce a power output of 50 MW with any combination of fuel oil and blast furnace gas (BFG). Only 10 units/h of BFG is available. Since the supply of BFG may not be sufficient for the required power generation, fuel oil must be purchased. It is desired to use the minimum amount of fuel oil in the two generators. Fuel requirements are expressed as a quadratic function of the power (MW) produced from a correlation:

$$f = a_0 + a_1 x + a_2 x^2$$

where x is power (MW) from each generator and f is fuel used (ton/h for fuel oil and units/f for BFG), with the constants for each generator given below.



	a_0	a_1	a_2
gen_1(oil)	1.4609	.15186	.00145
gen_1(gas)	1.5742	.16310	.001358
gen_2(oil)	0.8008	.20310	.000916
gen_2(gas)	0.7266	.22560	.000778

Assume that when a combination of fuel oil and BFG is used, the total power generated is summed. Power for first generator is from 18 to 30 MW while the second is 14 to 25 MW. Using the gams file **fueloil.gms,** go through the formulation of the problem. Identify the sets, variables, constraints and objective function. Also, note the special syntax of GAMS in referring to set indices.

a) What happens if gas supply increases from 10 to 15 units/h?
Can you predict this from the multipliers?

b) Suppose that fuel oil supply is restricted to 10 ton/h and BFG is to be purchased.
What is the minimum amount of BFG needed to supply the power requirement?