06-606

Assignment #6

Fall, 2011 Due: 11/18/11

1. Consider the nonconvex, constrained NLP:



Min (A + B)

$\left\{ x_{1}, y_{1} \geq R_{1} \right\}$	$x_1 \leq B - R_1, y_1 \leq A - R_1$
$\begin{cases} x_{2}, y_{2} \geq R_{2} \end{cases}$	$x_2 \leq B - R_2, \ y_2 \leq A - R_2$
$x_3, y_3 \ge R_3$	$x_3 \le B - R_3, y_3 \le A - R_3$

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:

Min x₂
s.t.
$$x_1 - x_2^2 + 1 \le 0$$

 $-x_1 - x_2^2 + 1 \le 0$

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

$$\mathbf{f}(\mathbf{x}) = [\mathbf{x}_1{}^2 + (\mathbf{x}_2{}{}{}^+ 1)^2][\mathbf{x}_1{}^2 + (\mathbf{x}_2{}{}^- 1)^2]$$

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. 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:

 $X7 = 86.35 + 1.098 \times X8 - 0.038 \times X8 \times 2 + 0.325 \times (X6-89.)$

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 fomulation. How would you interpret these results?

Adution - Honework 3

Consider NLP Min (A+B) x = 1, 3 $\varkappa_i, \gamma_i \gg k_i$ $\varkappa_i \neq B - R_i$ y: ≤ A - R: =0 $(\chi_i - \chi_j)^2 + (\chi_i - \chi_j)^2 > (R_i + R_j)^2$ Vitj KKT conditions Xi, yi > 0 are redundant and are o for xi & yi ! Mpi(xi-B+Ri) = 0 $\mu_{x_i}(y_i - A + R_i) = 0, \mu_{x_i}(R_i - x_i) = \mu_{y_i}(R_i - y_i) = 0$ -2(x,-x2) M12+2(x,-x3) M13 - M21 + MB1 = 0 i)-2 (x2-x) M12-2(x2-x3) H23 Mx2+ MB2 $-2(x_3-x_1)\mu_{13}-2(x_3-x_2)\mu_{23}-\mu_{*3}+\mu_{33}=0$ $-2(y_{1}-y_{2})\mu_{12}-2(y_{1}-y_{3})\mu_{13}-\mu_{y_{1}}+\mu_{A_{1}}=0$ $-2(y_{2}-y_{1})\mu_{12}-2(y_{2}-y_{3})\mu_{23}-\mu_{y_{2}}+\mu_{A2}=0$ $-2(y_{3}-y_{1})\mu_{13}-2(y_{3}-y_{2})\mu_{23}-\mu_{y_{3}}+\mu_{A3}=0$ \ddot{z} A & B " for 1 - (MAI + MAZ + MAZ) = 0 (ii)1 - (MBI + MBZ + MB3) = 0 $a_{lso}, \mu_{ij}((x_i - x_j)^2 + (y_i - y_j)^2 - (l_i^2 + l_j^2) = 0$ Nonconvedity - for quadratic constraints $g(x,y) = -(x^{2} + x^{2} - 2x^{2} + x^{2}) - (y^{2} + y^{2} - 2y^{2} + y^{2}) - (R^{2} + R^{2}) = 0$

2) -2 -2 -2 -2 sigenvalues of [-2 -2] are $(-2-\lambda)^2 - 4 = 4\lambda + \lambda^2 = 0$ $\lambda = 0, -4$ tilies matrix is negative semidefinite, hence not consep. from iii) we know at least one A and B. (i.e. $\chi_i = B - R_i, y_i = A - R_i$) ly adding up i) then Mx, + Mx2 + Mx3 = MB, + MB2 + MB3 = 1 and at least one circle must touch to x = 0 (i.e. $x_i = R_i$) by adding up ii) then and at least one circle must Touch y=O (ie.yi=Ri) M. Ri & A, Ri & B, MAINS = 0, My MA = 0 then if Mai > 0 or MBi 70, from

() e.g., 2(x; - x2) miz + 2(x, -x3) mi3 = MB, - Mx1 and 14:2 or 2+3 must touch lor both). if MB, > O X, > X2 or X, > X3 if Mx, >0 x2>x, or x3>x, semilar argument can be made for Ji) Mais Myi The problem has nonempre solutions, For example, if we interchange Zie Yi and A' B, the KT conditions are still satisfied. 2. Min X2 s.t. $\chi_1 - \chi_2^2 + 1 \le 0$ $-\chi_{1} - \chi_{2}^{2} + 1 \leq 0$ a) framble region b) Boch SGP TTTL and GRG start by lineaugung about $\chi^{\circ} = 0$. L'alus lineaugation $\Delta \chi \leq -1, \Delta \chi \geq 1$ is inconsistent 111 and both methods fail unless some "truck" is applied.

<pre>memark*(1.12+.12167*X8-0.0067*X8**2+0.325*(X6-89.)) ===86.35+1.098*X8**2+0.325*(X6-89.)) ===85.37-1.32 (**X2**1000*X3)===98000*X3/ **(X4*X7+1000*X3)===98000*X3/ **(X4*X7+1000*X3)===98000*X3/ **(X4*X7+1000*X3)===98000*X3/ **(X4*X7+5.04*X1-0.035*X2-10*X3-3.36*X5) = 0.063*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 1.22 = 0.063*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 1.22 = 0.053*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 0.063*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 0.063*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 1.22 = 0.063*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 0.063*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 1.22 = 0.063*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 1.22 = 0.063*X4*T7-5.04*X1-0.035*X2-10*X3-3.36*X5/ = 1.22</pre>	ALTIMITION FIGHERM FROM GIAD UDEA & LANDAL COMPLATION FILE = 0.000 SECONDS 0.8 Mb WIR205-130 1.0335 Rev 130 Windows RF193/99 3.14X1,MTON FROMEM FROM GIAD USER'S MANUAL LANCLATTON FROMEM FROM GIAD USER'S MANUAL MARCLATTON FROME AT 15 10 MARCLATTON FROME AT 12 2 MORE STANTISTICS BLOCKS OF PERMITTINS BLOCKS OF VARIABLES BLOCKS OF MARCLATION FROME AT 10 MINOS-130 GENERATION TIME BLOCKS OF MARCLATION FROME AT 10 MINOS-130 MINOS-130 GENERATION TIME BLOCKS OF MARCLATION FROME AT 10 MINOS-130 GENERATION FROME MARCLATION MINOS-130 MINOS-130 GENERATION TIME BLOCKS OF MARCLATION FROME AT 10 MINOS-130
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