1. Consider the nonconvex, constrained NLP:

Min \quad (A + B)

\begin{align*}
&x_1, y_1 \geq R_1 \quad x_1 \leq B - R_1, y_1 \leq A - R_1 \\
&x_2, y_2 \geq R_2 \quad x_2 \leq B - R_2, y_2 \leq A - R_2 \\
&x_3, y_3 \geq R_3 \quad x_3 \leq B - R_3, y_3 \leq A - R_3
\end{align*}

\text{no overlaps}

\begin{align*}
&\left((x_1 - x_2)^2 + (y_1 - y_2)^2 \geq (R_1 + R_2)^2\right) \\
&\left((x_1 - x_3)^2 + (y_1 - y_3)^2 \geq (R_1 + R_3)^2\right) \\
&\left((x_2 - x_3)^2 + (y_2 - y_3)^2 \geq (R_2 + R_3)^2\right)
\end{align*}

x_1, x_2, x_3, y_1, y_2, y_3, A, B \geq 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:

\[
\begin{align*}
\text{Min } & \quad x_2 \\
\text{s.t. } & \quad x_1 - x_2^2 + 1 \leq 0 \\
& \quad -x_1 - x_2^2 + 1 \leq 0
\end{align*}
\]

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. Consider the alkylation process shown below from Bracken & McCormick (1968)

\[
\begin{align*}
X_1 &= \text{Olefin feed (barrels per day)} \\
X_2 &= \text{Isobutane recycle (barrels per day)} \\
X_3 &= \text{Acid addition rate (1000s pounds/day)} \\
X_4 &= \text{Alkylate yield (barrels/day)} \\
X_5 &= \text{Isobutane input (barrels per day)} \\
X_6 &= \text{Acid strength (weight percent)} \\
X_7 &= \text{Motor octane number alkylate} \\
X_8 &= \text{External isobutane-to-olefin ratio} \\
X_9 &= \text{Acid dilution factor} \\
X_{10} &= \text{F-4 performance no. of alkylate}
\end{align*}
\]
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, $X_4$, is a function of both the olefin feed, $X_1$, and the external isobutane to olefin ratio, $X_8$. 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:

$$X_4 = X_1 \times (1.12 + 0.12167 \times X_8 - 0.0067 \times X_8^2)$$

The motor octane number of the alkylate, $X_7$, is a function of $X_8$ and the acid strength, $X_6$. The nonlinear regression under the same conditions as for $X_4$ yields:

$$X_7 = 86.35 + 1.098 \times X_8 - 0.038 \times X_8^2 + 0.325 \times (X_6 - 89.)$$

The acid dilution factor, $X_9$, can be expressed as a linear function of the F-4 performance number, $X_{10}$ and is given by:

$$X_9 = 35.82 - 0.222 \times X_{10}$$

Also, $X_{10}$ is expressed as a linear function of the motor octane number, $X_7$.

$$X_{10} = 3 \times X_7 - 133$$

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

$$X_8 = \frac{(X_2 + X_5)}{X_1}$$

To prevent potential zero divides it is rewritten as:

$$X_8 \times X_1 = X_2 + X_5$$

The isobutane feed, $X_5$, 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 $X_4 = X_1 + X_5 - 0.22 \times X_4$ or:

$$X_5 = 1.22 \times X_4 - X_1$$

Finally, the acid dilution strength ($X_6$) is related to the acid addition rate ($X_3$), the acid dilution factor ($X_9$) and the alkylate yield ($X_4$) by the equation, $1000 \times X_3 + X_4 \times X_6 \times X_9(98 - X_6)$. Again, we reformulate this equation to eliminate the division and obtain:

$$X_6 \times (X_r \times X_9 + 1000 \times X_3) = 98000 \times X_3$$
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)

\[
OBJ = 0.063 \times X4 \times X7 - 5.04 \times X1 - 0.035 \times X2 - 10 \times X3 - 3.36 \times X5
\]

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:

\[
0.99 \times X4 \leq RX4 \leq 1.01 \times X4
\]
\[
0.99 \times X7 \leq RX7 \leq 1.01 \times X7
\]
\[
0.99 \times X9 \leq RX9 \leq 1.01 \times X9
\]
\[
0.9 \times X10 \leq RX10 \leq 1.11 \times X10
\]

to allow for the relaxation. Resolve with this formulation. How would you interpret these results?
Consider NLP
\[ \text{Min} \ (A+B) \]
\[ s.t. \ z_i, y_i \geq 0, \ i = 1, 3 \]
\[ x_i \leq B - R_i \]
\[ y_i \leq A - R_i \leq 0 \]
\[ (x_i - x_j)^2 + (y_i - y_j)^2 \geq (R_i + R_j)^2 \quad \forall i \neq j \]

KKT conditions
- \( z_i, y_i \geq 0 \) are redundant and are always inactive
- For \( z_i \) and \( y_i \): \( \lambda_{z_i} (x_i - B + R_i) = 0 \)
  \( \lambda_{y_i} (y_i - A + R_i) = 0 \), \( \lambda_{z_i} (R_i - x_i) = \mu_{z_i} (R_i - y_i) = 0 \)
  i) \[-2 (x_1 - x_2) \mu_{12} + 2 (x_1 - x_3) \mu_{13} - \mu_{11} + \mu_{B1} = 0 \]
  \[-2 (x_2 - x_1) \mu_{12} - 2 (x_2 - x_3) \mu_{23} - \mu_{22} + \mu_{B2} = 0 \]
  \[-2 (x_3 - x_1) \mu_{13} - 2 (x_3 - x_2) \mu_{23} - \mu_{33} + \mu_{B3} = 0 \]
  ii) \[-2 (y_1 - y_2) \mu_{12} - 2 (y_1 - y_3) \mu_{13} - \mu_{y1} + \mu_{A1} = 0 \]
  \[-2 (y_2 - y_1) \mu_{12} - 2 (y_2 - y_3) \mu_{23} - \mu_{y2} + \mu_{A2} = 0 \]
  \[-2 (y_3 - y_1) \mu_{13} - 2 (y_3 - y_2) \mu_{23} - \mu_{y3} + \mu_{A3} = 0 \]

- For \( A + B \)
  iii) \[1 - (\mu_{A1} + \mu_{A2} + \mu_{A3}) = 0 \]
  \[1 - (\mu_{B1} + \mu_{B2} + \mu_{B3}) = 0 \]
  Also, \( \mu_{y} ((x_i - x_j)^2 + (y_i - y_j)^2) = (R_i + R_j)^2 = 0 \)
  a) Non convexity - for quadratic constraints
  \[ g(x, y) = -((x_i^2 + x_j^2 - 2x_i x_j) - (y_i^2 + y_j^2 - 2y_i y_j)) \]
  \[-(R_i^2 + R_j^2) \leq 0 \]
\[ \nabla^2 g = \begin{bmatrix} -2 & -2 \\ -2 & -2 \end{bmatrix} \]

eigenvalues of \[ \begin{bmatrix} -2 & -2 \\ -2 & -2 \end{bmatrix} \] are
\[ (-2 - \lambda)^2 - 4 = \lambda^2 + x^2 = 0 \]
\[ \lambda = 0, -4 \]

This matrix is negative semidefinite, hence not convex.

b) From iii), we know at least one circle \( \gamma \) must touch upper bounds \( A \) and \( B_i \) (i.e. \( x_i = \overline{B} - R_i, y_i = \overline{A} - R_i \))

By adding up i) then
\[ \mu_{x1} + \mu_{x2} + \mu_{x3} = \mu_{B1} + \mu_{B2} + \mu_{B3} = 1 \]
and at least one circle must touch \( \gamma \)
\[ x = 0 \] (i.e. \( x_i = R_i \))

By adding up ii) then
\[ \mu_{y1} + \mu_{y2} + \mu_{y3} = \mu_{A1} + \mu_{A2} + \mu_{A3} = 1 \]
and at least one circle must touch \( \gamma \)
\[ y = 0 \] (i.e. \( y_i = R_i \))

If \( x_i \leq A, R_i \leq B \), \( \mu_{x1} \mu_{x2} = 0, \mu_{y1} \mu_{y2} = 0 \)
otherwise if \( \mu_{x1} > 0 \) or \( \mu_{\beta_i} > 0 \), then
1) e.g.,
\[ 2(x_i - x_2) \mu_{12} + 2(x_1 - x_3) \mu_{13} = \mu_{13} - \mu_{12} \]
and 14.2 or 2+3 must touch (or both).

- If \( \mu_{13} > 0 \) \( x_1 > x_2 \) or \( x_1 > x_3 \)
- If \( \mu_{12} > 0 \) \( x_2 > x_1 \) or \( x_3 > x_1 \)

Similar argument can be made for \( y_i, \mu_{31}, y_3 \).

2) The problem has nonunique solutions. For example, if we interchange \( x_i \leftrightarrow y_i \) and \( A \leftrightarrow B \), the KKT conditions are still satisfied.

\[ \begin{align*}
\text{Min } x_2 \\
\text{s.t. } x_1 - x_2^2 + 1 &\leq 0 \\
- x_1 - x_2^2 + 1 &\leq 0
\end{align*} \]

a) Feasible region

b) Both SQP and GRG start by linearizing about \( x^0 = 0 \).

This linearization \( \Delta x_1 \leq -1 \), \( \Delta x_1 \geq 1 \) is inconsistent and both methods fail unless some "trick" is applied.
**Compilation Problem from GINO User's Manual**

**Compilation Time** = 0.000 seconds 0.8 Mb WIN205-130

**Model Statistics**
- Solving ALEY using NLP from line 58

**Model Summary**
- BLOCKS OF EQUATIONS: 8
- BLOCKS OF VARIABLES: 11
- NON ZERO ELEMENTS: 32
- DERIVATIVE POOL: 7
- CONSTANT POOL: 16
- CODE LENGTH: 132

**Generation Time** = 0.010 seconds 2.0 Mb WIN205-130

**Execution Time** = 0.010 seconds 2.0 Mb WIN205-130

<table>
<thead>
<tr>
<th>Model</th>
<th>ALEY</th>
<th>Objective OBJ</th>
<th>NLP</th>
<th>USE ( P(\text{SOLVER}) )</th>
<th>FROM LINE 58</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>SOLVER STATUS</strong></td>
<td>1 Normal Completion</td>
<td>2 Locally Optimal</td>
<td>931.1376</td>
<td></td>
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**Objective Value**: 931.1376

**Resource Usage Limit**: 0.020 1000.000

**Iteration Count Limit**: 20 1000

**Evaluation Errors**: 0 0

**COMOPT 3 Windows NT/95/98 version 2.071M-009-043**

**Using default control program.**

**Optimal solution. Reduced gradient less than tolerence.**

COMOPT time total: 0.008 seconds

of which: function evaluations: 0.000 = 0.8%
Derivative evaluations = 0.000 = 0.0%

Work length = 0.05 Mbytes
Estimate = 0.05 Mbytes
Max used = 0.04 Mbytes

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<th>MARGINAL</th>
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<td>57.425</td>
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<td>35.820</td>
</tr>
<tr>
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<td>-133.000</td>
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<tr>
<td>EQU E8</td>
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<th>MARGINAL</th>
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<td>VAR X3</td>
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<tr>
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<tr>
<td>VAR X6</td>
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<tr>
<td>VAR X7</td>
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<tr>
<td>VAR X8</td>
<td>3.08</td>
<td>9.357</td>
<td>12.00</td>
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ALKYATION PROBLEM FROM GING USER'S MANUAL

<table>
<thead>
<tr>
<th>LOWER</th>
<th>LEVEL</th>
<th>UPPER</th>
<th>MARGINAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>VAR X9</td>
<td>1.200</td>
<td>3.041</td>
<td>4.000</td>
</tr>
<tr>
<td>VAR X10</td>
<td>145.000</td>
<td>147.652</td>
<td>162.000</td>
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<tr>
<td>VAR OBJ</td>
<td>-INF</td>
<td>911.138</td>
<td>+INF</td>
</tr>
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</table>

*** REPORT SUMMARY: ***

0 MINDPT
0 INFEASIBLE
0 UNBOUNDED
0 ERRORS

EXECUTION TIME = 0.000 SECONDS 0.8 Mb WIN95-130

USER: Ignacio E. Grossmann
Carnegie Mellon University, Dept. of Chemical Engineering DC1272

*** FILE SUMMARY ***

INPUT: C:\DOCUMENTS AND SETTINGS\LORENS BIEGELS\DESKTOP\06-720\ALKY.GMS
OUTPUT: C:\DOCUMENTS AND SETTINGS\LORENS BIEGELS\DESKTOP\ALKY.LST
2
ALEXILATION PROBLEM FROM GINO USER'S MANUAL

1

59 X5.L = 0.174;
60 X3.L = 0.21;
61 X4.L = 0.179;
62 X5.L = 0.85;
63 X7.L = 0.36;
64 X6.L = 0.18;
65 X4.L = 0.2048;
67 X7.L = 0.93;
68 X5.L = 0.36;
69 X6.L = 0.18;
70 X10.L = 0.85;
72 73 SOLVE ALEX2 USING NLPS MAXIMIZING OBJ

1

COMPILATION TIME = 0.000 SECONDS 0.8 MB - WIN205-130

1

2

ALEXILATION PROBLEM FROM GINO USER'S MANUAL

Model Statistics
SOLVE ALEX2 USING NLPS FROM LINE 71

1

MODEL STATISTICS

BLOCKS OF EQUATIONS 16 SINGLE EQUATIONS 16
BLOCKS OF VARIABLES 15 SINGLE VARIABLES 15
ROW ZERO ELEMENTS 44 ROW LINEAR X = 11
DERIVATIVE POOL 7 CONSTANT POOL 16
CODE LENGTH 132

1

GENERATION TIME = 0.010 SECONDS 2.6 MB - WIN205-130

1

EXECUTION TIME = 0.010 SECONDS 2.6 MB - WIN205-130

1

2

ALEXILATION PROBLEM FROM GINO USER'S MANUAL

SOLVE SUMMARY

MODEL ALEX2 OBJECTIVE OBJ
TYPE NLPS DIRECTION MAXIMIZE
SOLVER CONCEPT FROM LINE 73

1

1

1

1

1

1

1

1

1

1

1
**EVALUATION ERRORS**

| Error | 0 | 0 |

**CONOPT 2** Windows NT/95/98 version 2.07LH-009-045
Copyright (C) ARKI Consulting and Development A/S
Bagsvaerdvej 266 A
DK-2880 Bagsvaerd, Denmark

Using default control program.

**Optimal solution. Reduced gradient less than tolerance.**

**CONOPT time**

- Total: 0.000 seconds
- Function evaluations: 0.000 = 0.0%
- Derivative evaluations: 0.000 = 0.0%

Work length = 0.05 Mbytes
Baseline = 0.05 Mbytes
Max used = 0.04 Mbytes

**LOWER** | **LEVEL** | **UPPER** | **MARGINAL**
--- | --- | --- | ---
**EQU E1** | 57.428 | 57.428 | 57.428 | 1.373
**EQU E2** | 57.428 | 57.428 | 57.428 | 443.509
**EQU E3** | 35.820 | 35.820 | 35.820 | -355.943
**EQU E4** | -133.000 | -133.000 | -133.000 | 78.933
**EQU E5** | -133.000 | -133.000 | -133.000 | 0.084
**EQU E6** | - | - | - | 0.001
**EQU E7** | - | - | - | 0.001
**EQU E8** | -INF | -64.973 | +INF | 0.001
**EQU E9** | -INF | -64.973 | +INF | 0.001
**EQU E10** | -INF | -64.973 | +INF | 0.001
**EQU E11** | -INF | -1.891 | +INF | 0.001
**EQU E12** | -INF | -1.891 | +INF | 0.001
**EQU E13** | -INF | -266.731 | +INF | 0.001
**EQU E14** | -INF | -266.731 | +INF | 0.001
**EQU E15** | -INF | -266.731 | +INF | 0.001
**EQU E16** | -INF | -266.731 | +INF | 0.001

**LARGE Rev 1.10** Windows NT/95/98

**VAR**

**LOWER** | **LEVEL** | **UPPER** | **MARGINAL**
--- | --- | --- | ---
**VAR X1** | 1923.693 | 2000.000 | 0.000
**VAR X2** | 16000.000 | 1923.693 | 0.000
**VAR X3** | 197.452 | 32520.000 | 0.000
**VAR X4** | 32520.000 | 32520.000 | 0.000
**VAR X5** | 2000.000 | 2000.000 | 0.000
**VAR X6** | 80.000 | 80.000 | 0.000
**VAR X7** | 90.000 | 90.000 | 0.000
**VAR X8** | 3.000 | 3.000 | 0.000
**VAR X9** | 3.000 | 3.000 | 0.000
**VAR X10** | 3.000 | 3.000 | 0.000
**VAR X11** | 3.000 | 3.000 | 0.000
**VAR X12** | 3.000 | 3.000 | 0.000
**VAR X13** | 3.000 | 3.000 | 0.000
**VAR X14** | 3.000 | 3.000 | 0.000
**VAR X15** | 3.000 | 3.000 | 0.000
**VAR X16** | 3.000 | 3.000 | 0.000

**REPORT SUMMARY**

- 0 **VAR**
- 1296.062 **INF**
- 0 **ERRORS**

**EXECUTION TIME**

- 0.000 seconds
- 0.6 MB
- WIN28S-130

**USER** Ignacio E. Grossmann
Carnegie Mellon University, Dept. of Chemical Engineering

**FILE SUMMARY**

- INPUT: C:\DOCUMENTS AND SETTINGS\LORENZ BIEGLER\DESKTOP\06.720\ALKYB.GMS
- OUTPUT: C:\DOCUMENTS AND SETTINGS\LORENZ BIEGLER\DESKTOP\ALKYB.LST