ECH4905 ChemE Optimization HW 6

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1 Problem 1

Consider the following problem:

$$\text{minimize} \begin{array}{l} Z_1(\mathbf{x}) = x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2, \\ Z_2(\mathbf{x}) = 3x_1 + 2x_2 - x_3^3 + 0.01(x_4 - x_5)^3, \end{array}$$

subject to:

$$\begin{aligned} x_1 + 2x_2 - x_3 - 0.5x_4 + x_5 &= 2, \\ 4x_1 - 2x_2 + 0.8x_3 + 0.6x_4 + 0.5x_5^2 &= 0, \\ x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 &\leq 10. \end{aligned}$$

1.1 Part A

Use the epsilon-constraint method to solve the above nonlinear programming (NLP) problem in GAMS. Upload your code.

Solution: To solve this with the epsilon-constraint method, we can take the first objective Z_1 and set that as our primary objective, while we take the second objective Z_2 and turn that into a constraint. The optimization problem now looks like this:

$$\begin{array}{rl} \text{minimize} & Z_1(\mathbf{x}) = x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 \\ \text{subject to} & x_1 + 2x_2 - x_3 - 0.5x_4 + x_5 = 2, \\ & 4x_1 - 2x_2 + 0.8x_3 + 0.6x_4 + 0.5x_5^2 = 0, \\ & x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 \leq 10 \\ & 3x_1 + 2x_2 - x_3^3 + 0.01(x_4 - x_5)^3 \leq \varepsilon \end{array}$$

Below is the GAMS code that was used for this problem.

```
Sets
n / 1*30 /;

Parameters
epsilon_n(n)
pareto_z1(n)
pareto_z2(n);
```

```
Scalars
    z2_min
    z2_max
    epsilon /1/;


Variables
x_1
x_2
x_3
x_4
x_5
z_1
z_2;

x_1.lo = -4;   x_1.up = 4;
x_2.lo = -4;   x_2.up = 4;
x_3.lo = 0;   x_3.up = 4;
x_4.lo = -4;   x_4.up = 4;
x_5.lo = -4;   x_5.up = 4;

z_1.lo = -1000; z_1.up = 1000;
z_2.lo = -1000; z_2.up = 1000;


Equations
z_1_eq
z_2_eq
constraint_1
constraint_2
constraint_3
non_neg_power_constraint
epsilon_constraint
;
z_1_eq.. z_1 =e= x_1**2 + x_2**2 + x_3**3 + x_4**2 + x_5**2;
z_2_eq.. z_2 =e= 3*x_1 + 2*x_2 - x_3**3 + 0.01*(x_4 - x_5)**3;
constraint_1.. x_1 + 2*x_2 - x_3 - 0.5*x_4 + x_5 =e= 2;
constraint_2.. 4*x_1 - 2*x_2 + 0.8*x_3 + 0.6*x_4 + 0.5*x_2**2 =e= 0;
constraint_3.. z_1 =l= 10;
non_neg_power_constraint.. x_4 =g= x_5;
epsilon_constraint.. z_2 =l= epsilon;

Model FullModel / all / ;
model BoundedModel / all - epsilon_constraint / ;

option NLP=baron;
option optcr = 0.00001;
```

```
option limrow = 4000;

* First, solve BoundedModel to get min and max z_2
solve BoundedModel using MINLP minimizing z_1;
z2_min = z_2.l;

solve BoundedModel using MINLP minimizing z_2;
z2_max = z_2.l;

* Now loop to build Pareto front
loop(n,
    epsilon_n(n) = z2_min + (z2_max - z2_min)*(ord(n)-1)/(card(n)-1);
    epsilon = epsilon_n(n);
    solve FullModel using MINLP minimizing z_1;
    pareto_z1(n) = z_1.l;
    pareto_z2(n) = z_2.l;
);

* Save results
execute_unload 'pareto_front.gdx', pareto_z1, pareto_z2, epsilon_n;
```

1.2 Part B

Create a plot with the Pareto front.
Solution: The plot is available in Figure 1

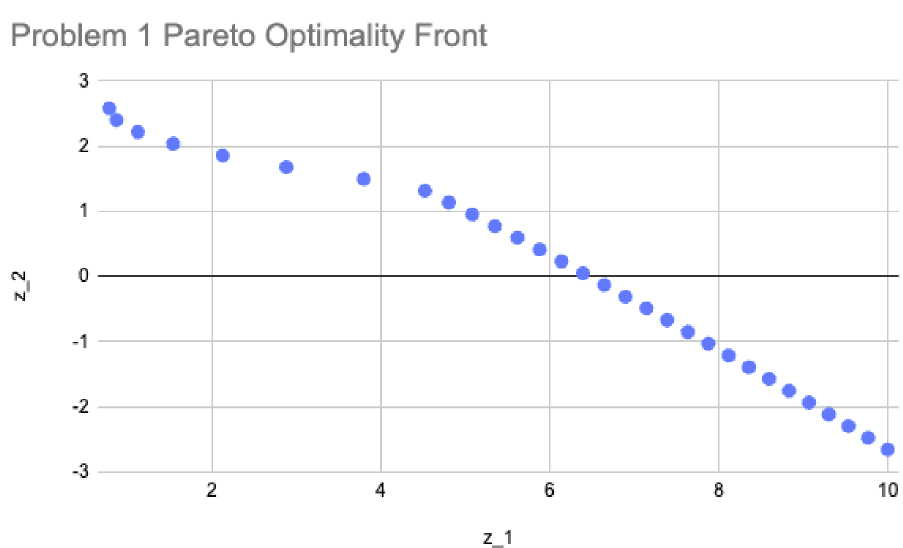

Figure 1: Problem 1 Pareto Chart

2 Problem 2

Consider the same problem that we explored in the previous homework in Figure 2.

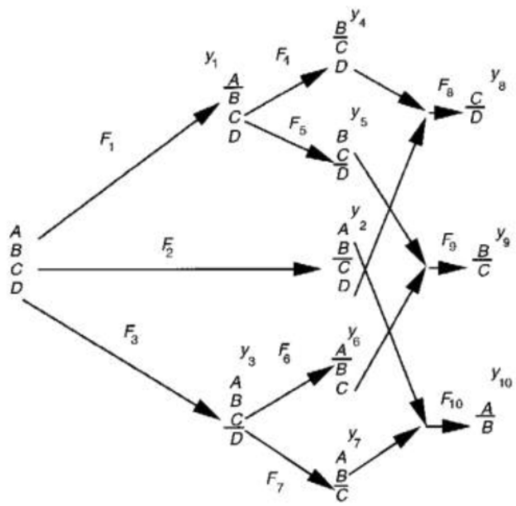

Figure 2: Problem 2 superstructure

In which the total cost of a distillation column was calculated as follows:

$$\text{cost}_k = \alpha_k + \beta_k F_k + \gamma_{\text{Hot}} Q_k^{\text{Hot}} + \gamma_{\text{Cold}} Q_k^{\text{Cold}},$$

where:

- α_k represents a fixed capital cost,
- β_k represents the variable investment cost,
- $\gamma_{\text{Hot}}/\gamma_{\text{Cold}}$ is the cost of hot/cold utilities,
- $Q_k^{\text{Hot}}/Q_k^{\text{Cold}}$ is the total demand of hot and cold utilities (assume they are equal).

Considering an initial feed of 1000 Kmol/h, and a composition of the feed stream (mole fraction) of $A = 0.15$, $B = 0.3$, $C = 0.35$, and $D = 0.2$, and the following data in Figure 3:

Scenario	Probability	γ_{Hot} (10^3 \$/10^6 KJ-y)	γ_{Cold} (10^3 \$/10^6 KJ-y)
1	0.025	0.1	3
2	0.05	0.1	10
3	0.1	0.1	34
4	0.15	1.3	3
5	0.35	1.3	10
6	0.15	1.3	34
7	0.1	3	3
8	0.05	3	10
9	0.025	3	34

Unlike the previous case, assume that the parameters γ_{Hot} and γ_{Cold} are known with uncertainty. The probability of occurrence in different scenarios is as follows:
Formulate a stochastic optimization problem in GAMS and solve the problem.

k	Separator	Investment cost α_k, fixed (10^3\$/yr)	β_k, variable (10^3\$hr/kmol yr)	Heat duty coefficients, K_k, (10^6kJ /kgmol)
1	*A/BCD*	145	0.42	0.028
2	*AB/CD*	52	0.12	0.042
3	*ABC/D*	76	0.25	0.054
6	*A/BC*	125	0.78	0.024
7	*AB/C*	44	0.11	0.039
4	*B/CD*	38	0.14	0.040
5	*BC/D*	66	0.21	0.047
10	*A/B*	112	0.39	0.022
9	*B/C*	37	0.08	0.036
8	*C/D*	58	0.19	0.044

Cost of utilities:

Cooling water $C_C = 1.3$ (10^3\$/10^6kJyr)
Steam $C_H = 34$ (10^3\$/10^6kJyr)

Figure 3: Problem 2 Data table

Solution:

$$\text{minimize} \quad \sum_{s\in S} p_s \cdot \left(\sum_{k=1}^{10} \left(\alpha_k y_k + \beta_k x_k + \gamma_{\text{Hot},s} Q_k^{\text{Hot}} + \gamma_{\text{Cold},s} Q_k^{\text{Cold}} \right) \right)$$

subject to:

Flow balance constraints (as defined in the problem)
Binary constraints for y variables
Big-M constraints for x variables
Supply and demand constraints
Non-negativity constraints for x variables.

We can rearrange the summations

$$\text{minimize} \quad \sum_{k=1}^{10} (\alpha_k y_k + \beta_k x_k) + \sum_{s\in S} p_s \cdot \sum_{k=1}^{10} \left(\gamma_{\text{Hot},s} Q_k^{\text{Hot}} + \gamma_{\text{Cold},s} Q_k^{\text{Cold}} \right)$$

Previously, in HW5 I didn't successfully incorporate the Q and γ values. Here, the γ values are provided per scenario. I believe the Q values are equal to the amount of flow passing through the distillation column times the heat duty coefficients. So, using the same variables y and x per distillation column that I had previously, we have the below full problem:

$$\text{minimize} \quad \sum_{k=1}^{10} (\alpha_k y_k + \beta_k x_k) + \sum_{s\in S} p_s \cdot \sum_{k=1}^{10} \left(\gamma_{\text{Hot},s} K_k x_k + \gamma_{\text{Cold},s} K_k x_k \right)$$

subject to:

Flow balance constraints (as defined in the problem)

Binary constraints for y variables

Big-M constraints for x variables

Supply and demand constraints

Non-negativity constraints for x variables.

There are no constraints affected by the uncertainty in the γ values. Therefore, we solve the same problem as previously but augment the objective function to include this uncertainty. For simplicity, we also split the first section $\sum_{k=1}^{10}(\alpha_k y_k + \beta_k x_k)$ into z_1 as the first stage component and the rest $\sum_{s\in S} p_s \cdot \sum_{k=1}^{10}(\gamma_{\text{Hot},s} K_k x_k + \gamma_{\text{Cold},s} K_k x_k)$ as the second stage component z_2. Now, $z_T = z_1 + z_2$ is the total objective component.

Another rearrangement we do for simplicity is factoring out the Kx term in the second stage component.

$$\text{minimize} \quad \sum_{k=1}^{10}(\alpha_k y_k + \beta_k x_k) + \sum_{k=1}^{10} K_k x_k \sum_{s\in S} p_s \cdot (\gamma_{\text{Hot},s} + \gamma_{\text{Cold},s})$$

Since this parameter $\sum_{s\in S} p_s \cdot (\gamma_{\text{Hot},s} + \gamma_{\text{Cold},s})$ is only comprised of parameters, we can actually calculate a new parameter as the expectation of this term. Instead of incorporating this into the GAMs, I created a new parameter $E[\gamma] = \sum_{s\in S} p_s \cdot (\gamma_{\text{Hot},s} + \gamma_{\text{Cold},s})$ and use that to solve the stochastic program below

$$\text{minimize} \quad \sum_{k=1}^{10}(\alpha_k y_k + \beta_k x_k) + \sum_{k=1}^{10} K_k x_k E[\gamma]$$

subject to:

Flow balance constraints (as defined in the problem)

Binary constraints for y variables

Big-M constraints for x variables

Supply and demand constraints

Non-negativity constraints for x variables.