# 054402 Design and Analysis

## LECTURE FOUR

## Constrained Optimization

Refs: Seider, Seader and Lewin (2004), Chapter 18
Edgar, Himmelblau, Lasdon (2001), Chapter 9
Reklaitis, Ravindran and Ragsdell (1983), Section 11.1



## OBJECTIVES

On completion of this course unit, you are expected to be able to:

- Formulate a general nonlinear program (NLP) to optimize a process using equality and inequality constraints
- Formulate and solve a linear program (LP)
- Formulate and solve a mixed integer linear program (MILP) using the branch-and-bound method.

## THE NONLINEAR PROGRAM (NLP)

- Formulation begins with the steady-state simulation of the process flowsheet, for a nominal set of specifications or design variables:

$$N_V = N_E + N_D$$

- The $N_D$ design variables are first set using heuristics, and latter adjusted to better achieve design objectives (optimized)
- During this process, the models used are improved and refined, property prediction methods tuned, and profitability measures are computed
- The NLP is then formulated, consisting of:
  - Objective function to be minimized
  - Subject to: equality and inequality constraints



## OBJECTIVE FUNCTION

Candidates for the measure of goodness of a design, f(d), where d is a vector of $N_D$ design variables are approximate profitability measures:

- ROI – Return of Investment (max)
- VP – Venture Profit (max)
- PBP – Payback period (min)
- $C_A$ -Annualized Cost (min)

or more rigorous measures

NPV – Net present value (max)

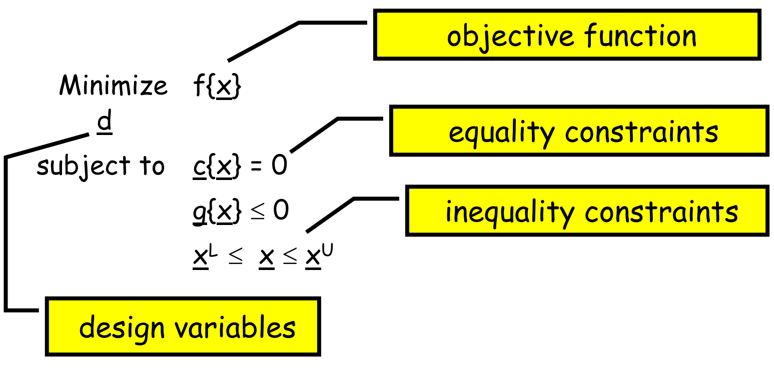
IRR – Investors rate of return (max)

## EQUALITY/INEQUALITY CONSTRAINTS

- In process simulators, most of the equality constraints, $\underline{c}\{\underline{x}\} = 0$, are the model equations relating to M&E balances. These are not stated explicitly, but are invoked as each unit operation is installed on the flowsheet
- Some equality constraints are due to performance specifications (e.g., 95% recovery of species i in the distillate flow: $x_i D - 0.95 z_i F = 0$)
- A major advantage of using simulators is the ease with which inequality constraints, $\underline{g}\{\underline{x}\} \leq 0$, can be introduced, to bound the feasible region of operation (e.g., at least 95% recovery is specified by: $x_i D - 0.95 z_i F \geq 0$)

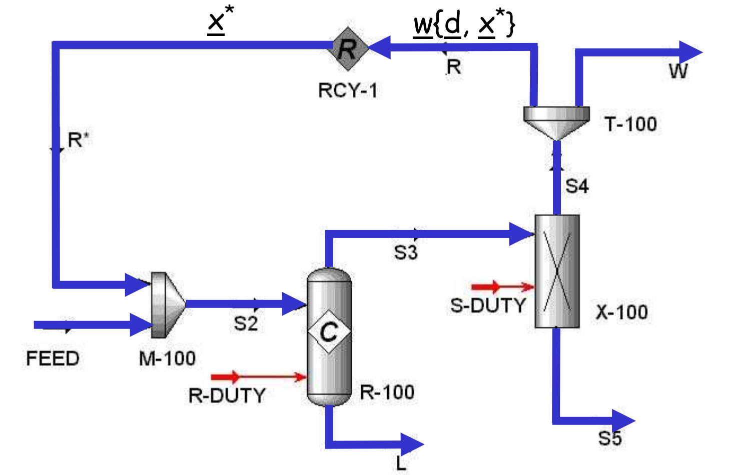


## THE NONLINEAR PROGRAM (NLP)




The $N_D$ design variables, $\underline{d}$, are adjusted to minimize $f\{\underline{x}\}$ while satisfying the constraints

## DEALING WITH RECYCLE STREAMS




Tear equations: $\underline{h}\{\underline{d}, \underline{x}^*\} = \underline{x}^* - \underline{w}\{\underline{d}, \underline{x}^*\} = 0$



## OPTIMIZATION ALGORITHM

Minimize over $\underline{d}$: $f\{\underline{x}, \underline{d}\}$ — objective function

Subject to: $\underline{h}\{\underline{x}^*, \underline{d}\} = \underline{x}^* - \underline{w}\{\underline{x}^*, \underline{d}\} = 0$ — tear equations

$\underline{c}\{\underline{x}, \underline{d}\} = 0$ — equality constraints

$\underline{g}\{\underline{x}\} \leq 0$ — inequality constraints

$\underline{x}^L \leq \underline{x} \leq \underline{x}^U$

$\underline{d}$ — design variables

## REPEATED SIMULATION

Minimize $f\{\underline{x}, \underline{d}\}$ over $\underline{d}$

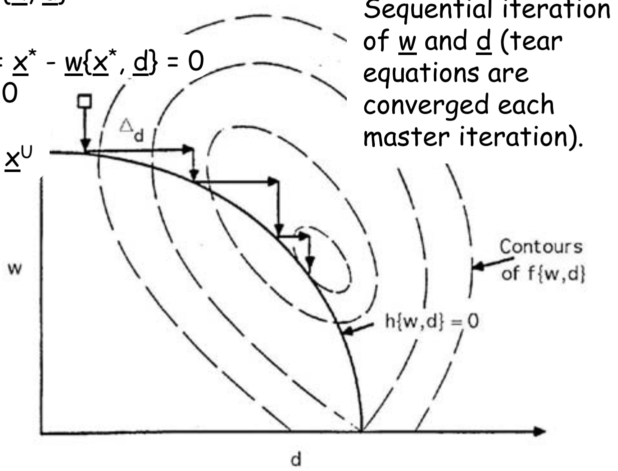
S.t. $\underline{h}\{\underline{x}^*, \underline{d}\} = \underline{x}^* - \underline{w}\{\underline{x}^*, \underline{d}\} = 0$

$\underline{c}\{\underline{x}, \underline{d}\} = 0$

$\underline{g}\{\underline{x}\} \leq 0$

$\underline{x}^L \leq \underline{x} \leq \underline{x}^U$

Sequential iteration of $\underline{w}$ and $\underline{d}$ (tear equations are converged each master iteration).






## INFEASIBLE PATH APPROACH (SQP)

Minimize $f\{\underline{x}, \underline{d}\}$ over $\underline{d}$

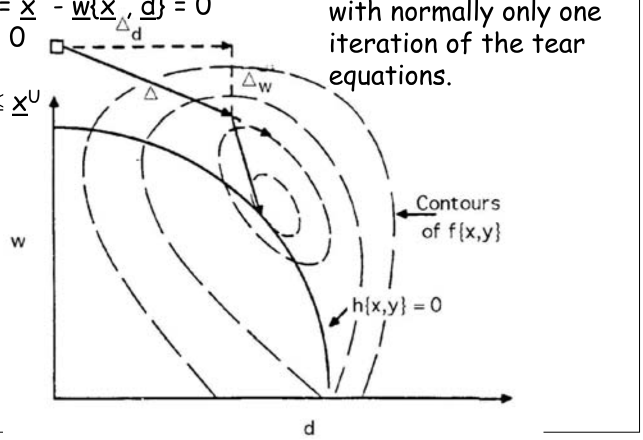
S.t. $\underline{h}\{\underline{x}^*, \underline{d}\} = \underline{x}^* - \underline{w}\{\underline{x}^*, \underline{d}\} = 0$

$\underline{c}\{\underline{x}, \underline{d}\} = 0$

$\underline{g}\{\underline{x}\} \leq 0$

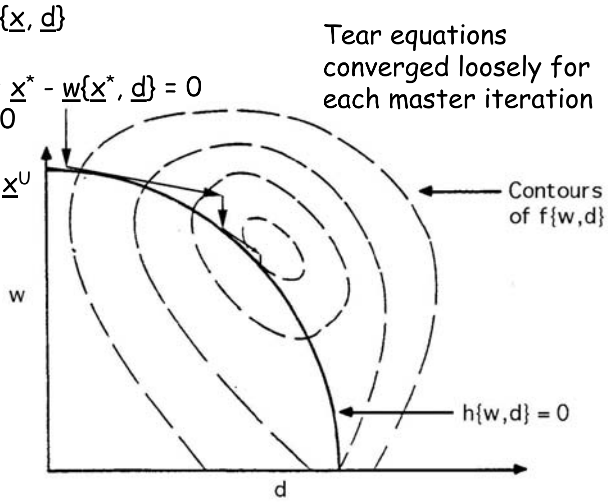
$\underline{x}^L \leq \underline{x} \leq \underline{x}^U$

Both $\underline{w}$ and $\underline{d}$ are adjusted simultaneously, with normally only one iteration of the tear equations.



## COMPROMISE APPROACH (SQP)

Minimize $f\{\underline{x}, \underline{d}\}$
$\underline{d}$
S.t. $\underline{h}\{\underline{x}^*, \underline{d}\} = \underline{x}^* - \underline{w}\{\underline{x}^*, \underline{d}\} = 0$
$\underline{c}\{\underline{x}, \underline{d}\} = 0$
$\underline{g}\{\underline{x}\} \leq 0$
$\underline{x}^L \leq \underline{x} \leq \underline{x}^U$






## PRACTICAL ASPECTS

- Design variables, need to be identified and kept free for manipulation by optimizer
  - e.g., in a distillation column, reflux ratio specification and distillate flow specification are degrees of freedom, rather than their actual values themselves
- Design variables should be selected AFTER ensuring that the objective function is sensitive to their values
  - e.g., the capital cost of a given column may be insensitive to the column feed temperature
- Do not use discrete-valued variables in gradient-based optimization as they lead to discontinuities in $\underline{f}(\underline{d})$
- More info: See Chapter 18 and the Multimedia.

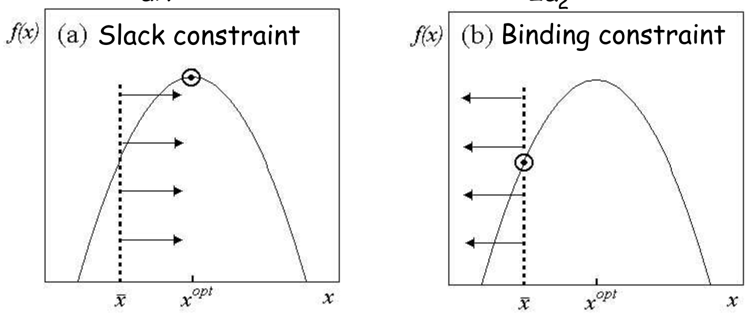
## NONLINEAR INEQUALITY CONSTRAINTS

- Consider the quadratic objective:

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

- The maximum is found by differentiation:

$$\frac{df}{dx} = 0 = a_1 + 2a_2 x \Rightarrow x_{opt} = -\frac{a_1}{2a_2}$$

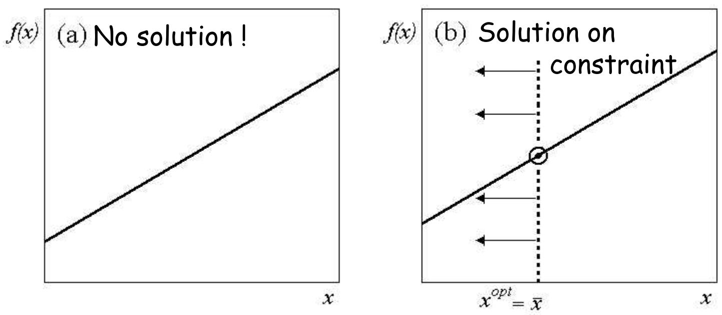





## LINEAR INEQUALITY CONSTRAINTS

- Consider the linear objective:

$$f = a_0 + a_1 x$$




- Now consider the constraint: $x \le \bar{x}$

## LINEAR PROGRAMING (LP)

$$\underset{\underline{d}}{\text{Minimize}}\ J\{\underline{x}\} = \sum_{i=1}^{N_v} f_i\, x_i$$ — objective function

Subject to (s.t.) $x_i \ge 0, i = 1,\ldots,N_V$

$$\sum_{j=1}^{N_v} a_{ij} x_j = b_i, i = 1,\ldots,N_E$$ — equality constraints

$$\sum_{j=1}^{N_v} c_{ij} x_j \le d_i, i = 1,\ldots,N_I$$ — inequality constraints

design variables

The $N_D$ design variables, $\underline{d}$, are adjusted to minimize $f\{\underline{x}\}$ while satisfying the constraints

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## EXAMPLE LP – GRAPHICAL SOLUTION

A refinery produces two crude oils, with yields as below.

| | Volumetric Yields | | Max. Production |
|---|---|---|---|
| | Crude #1 | Crude #2 | (bbl/day) |
| Gasoline | 70 | 31 | 6,000 |
| Kerosene | 6 | 9 | 2,400 |
| Fuel Oil | 24 | 60 | 12,000 |

The profit on processing each grade is:
$2/bbl for Crude #1 and $1.4/bbl for Crude #2.

a) What is the optimum daily processing rate for each grade?

b) What is the optimum if 12,000 bbl/day of gasoline is needed?

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## EXAMPLE LP – SOLUTION (Cont'd)

Step 1. Identify the variables. Let $x_1$ and $x_2$ be the daily production rates of Crude #1 and Crude #2.

Step 2. Select objective function. We need to <u>maximize</u> profit: $J\{\underline{x}\} = 2.00x_1 + 1.40x_2$

Step 3. Develop models for process and constraints. Only constraints on the three products are given:

$$0.70x_1 + 0.31x_2 \le 6{,}000$$
$$0.06x_1 + 0.09x_2 \le 2{,}400$$
$$0.24x_1 + 0.60x_2 \le 12{,}000$$

Step 4. Simplification of model and objective function. Equality constraints are used to reduce the number of independent variables ($N_D = N_V - N_E$). Here $N_E = 0$.

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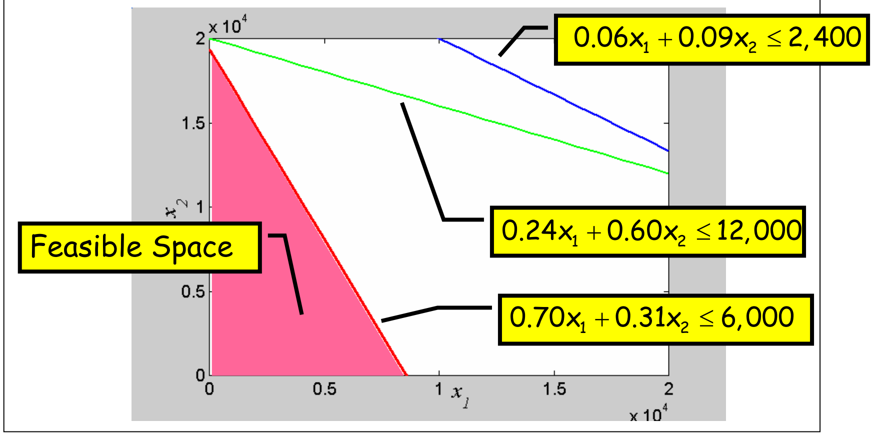
## EXAMPLE LP – SOLUTION (Cont'd)

Step 5. Compute optimum.

a) Inequality constraints define feasible space.

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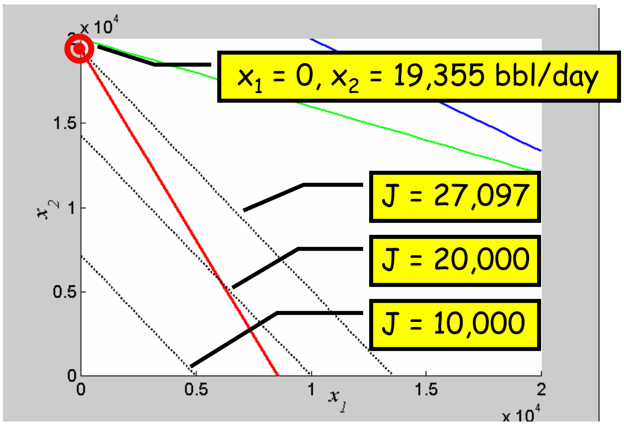
## EXAMPLE LP – SOLUTION (Cont'd)

Step 5. Compute optimum.

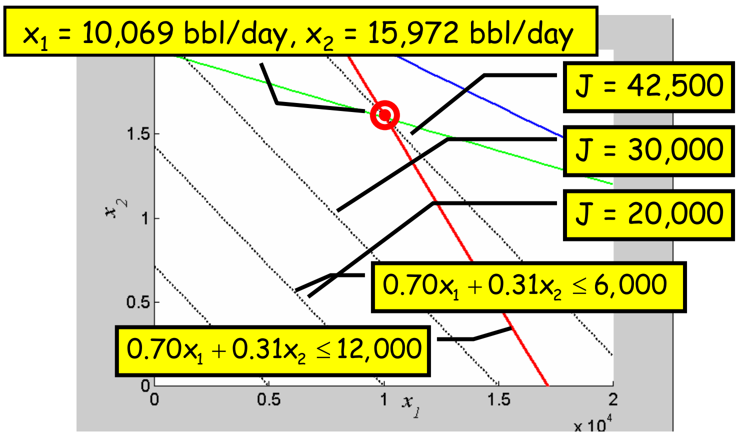
b) Constant J contours are positioned to find optimum.






## EXAMPLE LP – SOLUTION (Cont'd)

Step 5. Compute optimum – Gasoline demand doubles.



## MIXED INTEGER LINEAR PROGRAMING (MILP)

$$\underset{\underline{d}}{\text{Minimize}}\, J\{\underline{x},\underline{y}\} = \sum_{j=1} f_j x_j + \sum_{j=1} g_j y_j$$ — objective function

Subject to (s.t.) $x_j \geq 0, j = 1,\ldots,N_V$ — some could be integer

$$\sum_{j=1}^{N_V} a_{ij} x_j = b_i, i = 1,\ldots,N_E$$ — equality constraints

$$\sum_{j=1}^{N_V} c_{ij} x_j \leq d_i, i = 1,\ldots,N_I$$ — inequality constraints

$y_j \in (0,1)$ — binary variables

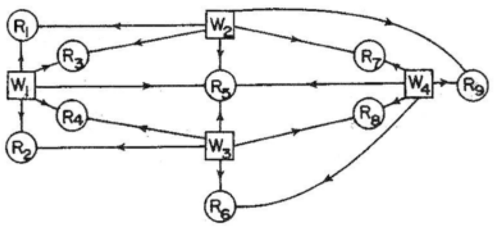
design variables

The design variables, $\underline{d}$, are adjusted to minimize $J\{\underline{x}, \underline{y}\}$ while satisfying the constraints



## EXAMPLE MILP FORMULATION

A firm has 4 possible sites for locating warehouses. The cost of locating a warehouse at site i is $K. There are 9 retail outlets, and each must be supplied by at least one warehouse. As shown below, it is not possible for one site to supply all of the retail outlets.




Formulate a MIP problem, whose solution is the location of warehouses to minimize costs.

Let decision variables be $y_i$ = 1 if we locate warehouse i.

## EXAMPLE MILP FORMULATION



## EXAMPLE MILP – BRANCH & BOUND SOLUTION

Solve the following MILP, noting that $x_1$ and $x_2$ are integers.

$$\underset{x_1,x_2}{\text{Maximize}}\ J\{\underline{x}\} = 3x_1 + 2x_2$$

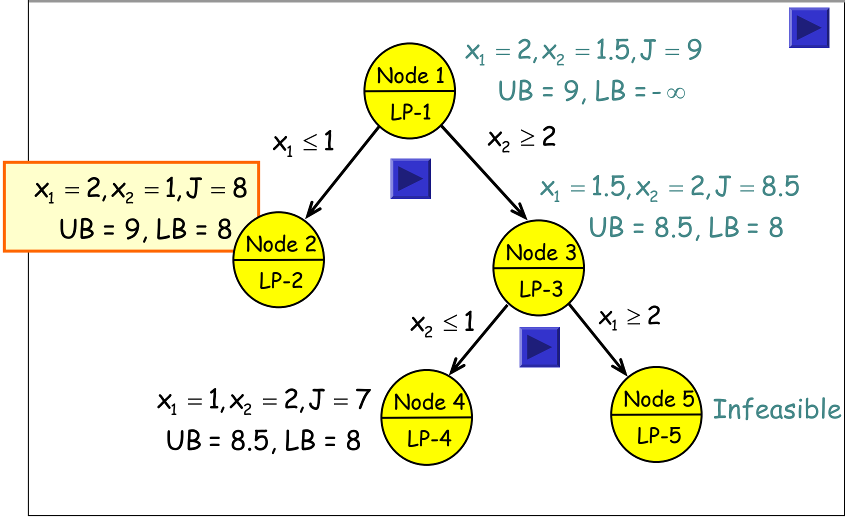
$$\text{Subject to}\ \ x_1 \le 2$$

$$x_2 \le 2$$

$$x_1 + x_2 \le 3.5$$

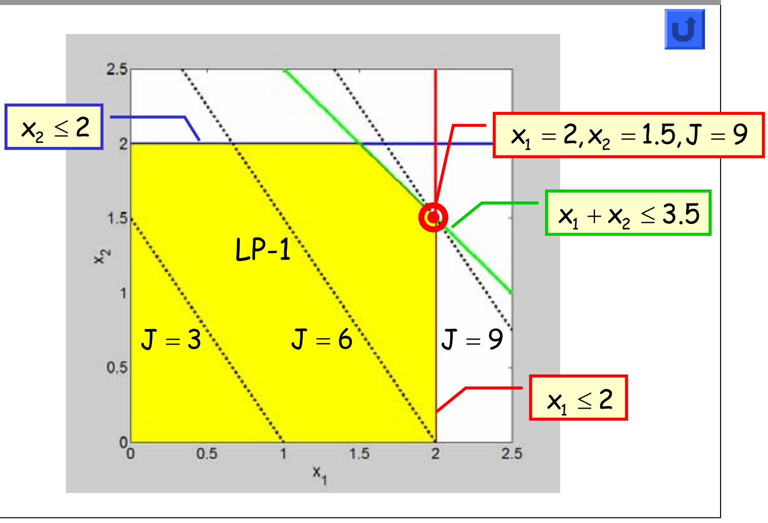
$$x_1, x_2 \ge 0 \text{ and integral}$$

## EXAMPLE MILP – BRANCH & BOUND SOLUTION






## EXAMPLE MILP – BRANCH & BOUND SOLUTION



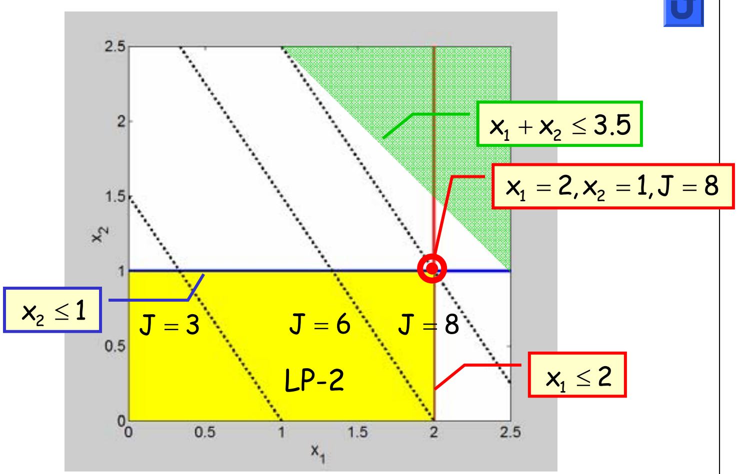
## EXAMPLE MILP – BRANCH & BOUND SOLUTION

Branch on $x_2$

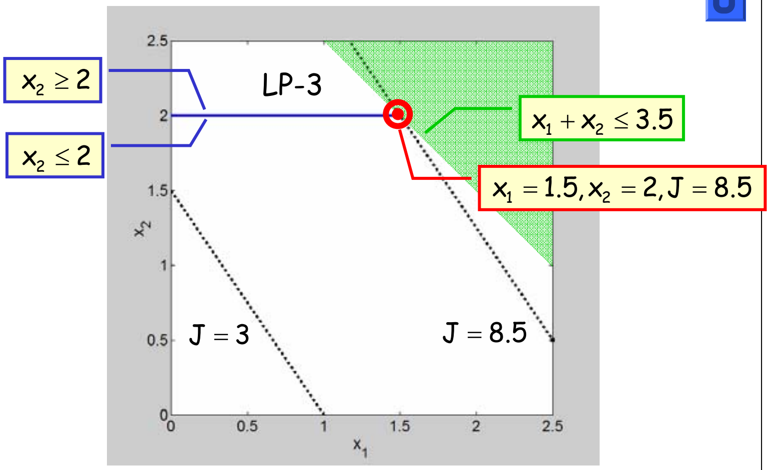
| LP-2 | LP-3 |
|---|---|
| $\underset{x_1,x_2}{\text{Maximize}}\ J\{\underline{x}\} = 3x_1 + 2x_2$ | $\underset{x_1,x_2}{\text{Maximize}}\ J\{\underline{x}\} = 3x_1 + 2x_2$ |
| Subject to $x_1 \le 2$ | Subject to $x_1 \le 2$ |
| $x_2 \le 2$ | $x_2 \le 2$ |
| $x_1 + x_2 \le 3.5$ | $x_1 + x_2 \le 3.5$ |
| (new constraint) $x_2 \le 1$ | (new constraint) $x_2 \ge 2$ |
| $x_1, x_2 \ge 0$ | $x_1, x_2 \ge 0$ |



## EXAMPLE MILP – BRANCH & BOUND SOLUTION



## EXAMPLE MILP – BRANCH & BOUND SOLUTION

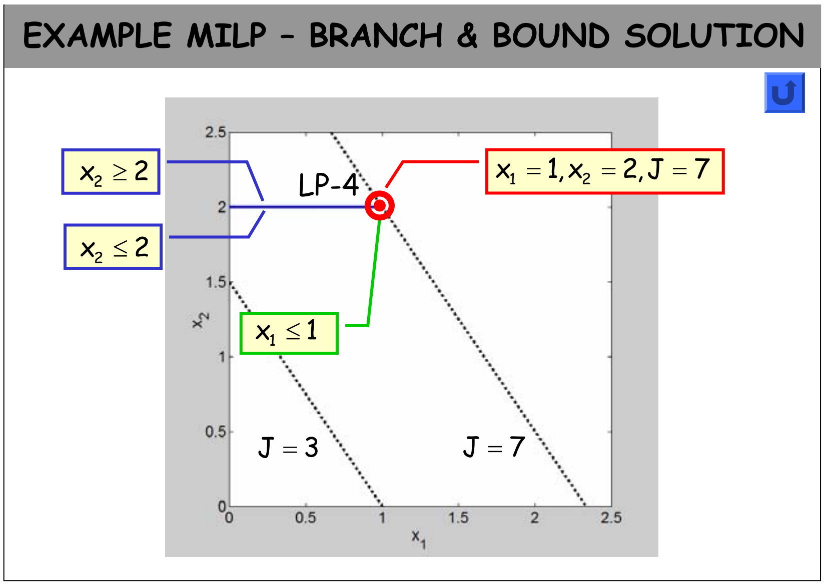





## EXAMPLE MILP – BRANCH & BOUND SOLUTION

Branch on $x_1$

| LP-4 | LP-5 |
|---|---|
| $\underset{x_1,x_2}{\text{Maximize}}\ J\{\underline{x}\} = 3x_1 + 2x_2$ | $\underset{x_1,x_2}{\text{Maximize}}\ J\{\underline{x}\} = 3x_1 + 2x_2$ |
| Subject to $x_1 \leq 2$ | Subject to $x_1 \leq 2$ |
| $x_2 \leq 2$ | $x_2 \leq 2$ |
| $x_1 + x_2 \leq 3.5$ | $x_1 + x_2 \leq 3.5$ |
| (From LP-3) $x_2 \geq 2$ | (From LP-3) $x_2 \geq 2$ |
| (new constraint) $x_1 \leq 1$ | (new constraint) $x_1 \geq 2$ |
| $x_1, x_2 \geq 0$ | $x_1, x_2 \geq 0$ |

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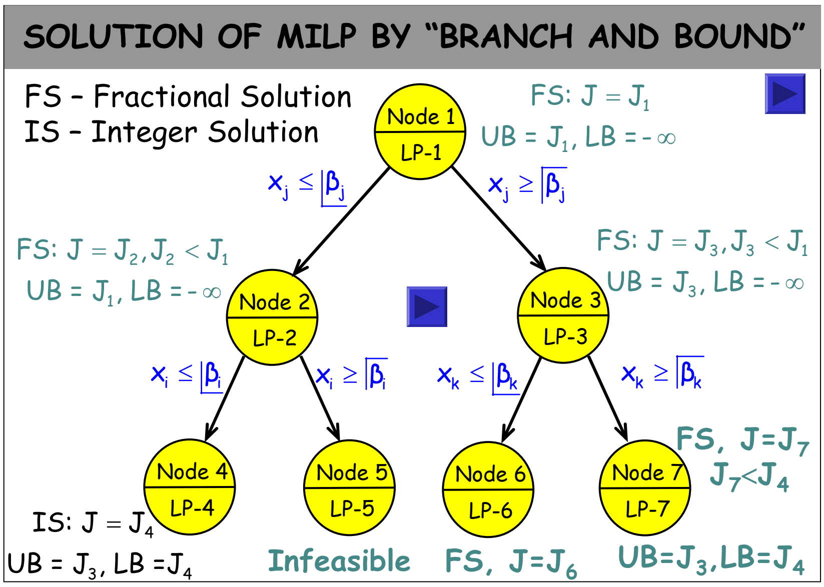


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## SOLUTION OF MILP BY "BRANCH AND BOUND"

1. Solve the MILP as an LP (ignore integer restrictions). If the result of LP-1, $J_1$, does not contain fractions in place of integers, this is the solution (END).
2. If not, J1 is the infeasible upper bound (UB) to the solution. Partition the feasible region of LP-1 by branching on one of the integer variables at a fractional value, selected using one of these rules:
   - o Select integer variable with the largest fractional value in the LP solution
   - o Branch on the most important variable first
3. Suppose we select variable $x_j$ for further branching. We create two new LP problems LP-2 and LP-3, by introducing constraints $x_j \le \lfloor \beta_j \rfloor$ and $x_j \ge \lceil \beta_j \rceil$ .



## SOLUTION OF MILP BY "BRANCH AND BOUND"

Branch on $x_j$

| LP-2 | LP-3 |
|---|---|
| Maximize $J = \underline{f}\underline{x}$ | Maximize $J = \underline{f}\underline{x}$ |
| Subject to $\underline{\underline{A}}\underline{x} \le \underline{b}$ | Subject to $\underline{\underline{A}}\underline{x} \le \underline{b}$ |
| (new constraint) $x_j \le \lfloor \beta_j \rfloor$ | (new constraint) $x_j \ge \lceil \beta_j \rceil$ |
| $\underline{x} \ge 0$ | $\underline{x} \ge 0$ |

## SOLUTION OF MILP BY "BRANCH AND BOUND"

4. Suppose both LP-2 and LP-3 are fractional, and hence infeasible to the MILP problem with integer restrictions.
5. The next step is to select either LP-2 or LP-3 and branch from that by adding a new constraint. A number of rules have been proposed on how to select the proper node for branching:
   - o Select LP with the largest value (for maximization)
   - o Select LP problem solved most recently (arbitrary)
6. Continue this procedure until node is **fathomed:** (a) Feasible integer solution; (b) LP infeasible; (c) Optimal value found < current lower bound.



## CONSTRAINED OPTIMIZATION - SUMMARY

On completion of this course unit, you are expected to be able to:

- Formulate a nonlinear program (NLP) to optimize a process using equality and inequality constraints.
- Formulate and solve a linear program (LP) and a mixed integer linear program (MILP). For a system involving two decision variables, you should be able to solve these graphically.
- Be able to optimize a process using HYSYS beginning with the results of a steady-state simulation

To work efficiently, it is recommended that sensitivity analysis on the objective function and constraints be carried before invoking the automated NLP solvers.