Linear Programming (LP): Formulating Models for LP

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ChE 4G03: Optimization in Chemical Engineering

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LP: Model Formulation

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"Straightforward" Models for LP

Approximations and Reformulations as LP Models

Outline

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"Straightforward" LP Models Formulation

Everything in life is **not linear and continuous**! But an enormous variety of applications can be modeled validly as LPs:

- Allocation Models
- Blending Models
- Operations Planning
- Operations Scheduling

For additional examples, see Rardin (1998), Chapter 4

Allocation Models

The main issue in allocation models is to divide or allocate a valuable resource among competing needs.

- The resource may be land, capital, time, fuel, or anything else of limited availability
- Principal decision variables in allocation models specify how much of the critical resource is allocated to each use

Example:

The Ontario Forest Service must trade-off timber, grazing, recreational, environmental, regional preservation and other demands on forestland.

The optimization seeks the best possible allocation of land to particular prescriptions (e.g., in terms of the *net present value*), subject to forest-wide restrictions on land use.

 $x_{i,j} \stackrel{\Delta}{=}$ number of acres in area i managed by prescription j

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Blending Models

The main issue in blending models is to decide what mix of ingredients best fulfills specified output requirements.

- The blend can be from chemicals, diets, metals, animal foods, etc.
- Principal decision variables in blending models specify how much of the available ingredients to include in the mix
- Composition constraints typically enforce lower and/or upper limits on the properties of the blend

Example: Gasoline Blending Process

Maximize: Profit

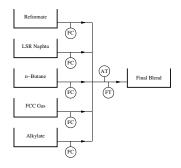
Subject to: Product Flow = ●

 \bullet < Octane No. < \bullet

 $\bullet < \mathsf{RVP} < \bullet$

• < Rel. Vol. < •

• < Component Flows < •



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Operations Planning Models

The main issue in operations planning models is to help a decision maker decide what to do and where to do it.

- The decision making can be in manufacturing, distribution, government, volunteer, etc.
- Principal decision variables in operations planning always resolve around what operations to undertake — recall that, to gain tractability, decision variables of relatively large magnitude are best modeled as continuous
- Balance constraints assure that in-flows equal or exceed out-flows for materials and products created by one stage of production and consumed by others

Example: Which amounts of Feed 1 and Feed 2 should we use?



Operations Planning Models

Class Exercise: What is the Optimization Model?

| | Prod. 1 | Prod. 2 | Prod. 3 | Feed Min. | Feed Max. | Feed Cost |
|-------------|---------|---------|---------|-----------|-----------|-----------|
| Feed 1 | 0.7 | 0.2 | 0.1 | 0 | 1000 | 5 |
| Feed 2 | 0.2 | 0.2 | 0.6 | 0 | 1000 | 6 |
| Prod. Min. | 0 | 0 | 0 | | | |
| Prod. Max. | 100 | 70 | 90 | | | |
| Prod. Value | 10 | 11 | 12 | | | |

Operations Scheduling Models

In operations scheduling models, the work is already fixed and the resources must be planned for meeting varying-time demands.

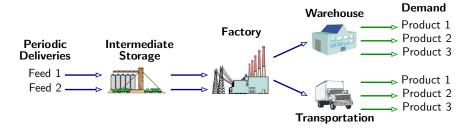
- Principal decision variables in operations scheduling are time-phased — time is an index and decisions may be repeated in each time period
 - Number of ball-bearings produced during period t
 - ▶ Inventory level at the beginning of period t
 - ▶ Number of employees beginning a shift at time t
- Scheduling models typically link decisions in successive time periods with balance constraints of the form:

$$\begin{pmatrix} \text{starting} \\ \text{level in} \\ \text{period } t \end{pmatrix} + \begin{pmatrix} \text{impacts of} \\ \text{period } t \\ \text{decisions} \end{pmatrix} = \begin{pmatrix} \text{starting} \\ \text{level in} \\ \text{period } t+1 \end{pmatrix}$$

• Covering constraints assure that the requirements over each time periods are met

Operations Scheduling Models

Example: Raw material deliveries are now periodic: We must decide when and how much raw materials to purchase in order to maximize profit while satisfying the demand



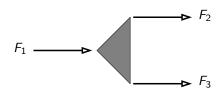
- The model must consider the inventories in tanks, factory, warehouses
- Delays in transportation can be important
- What type of balances are needed?

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Formulating "Straightforward" Models for LP

Example: Flow Splitting



Feed and product mole fractions $\alpha_1, \ldots, \alpha_n$

Material Balance:

$$F_1 = F_2 + F_3$$

• Feed and product composition (mole fractions) cannot change — Why?

"Straightforward" Models for LP

Fundamental Balances:

• Material: ball bearings, fluid, people, etc.

• Energy: vehicle travel, processing, etc.

• Space: volume, area

• Lumped quantity: pollution, economic activity, etc.

• Time: utilization of equipment, people work, etc.

Only retain key decisions as variables:

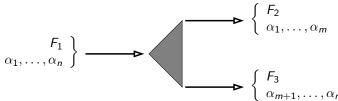
- Production rates
- Flows
- Investment
- Inventories

Combine other factors in parameters (constants)

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Formulating "Straightforward" Models for LP

Example: Perfect Separator



Material Balance:

$$F_1 = F_2 + F_3$$

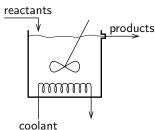
Component Balance:

$$F_1 \sum_{k=1}^{m} \alpha_m = F_2$$

- Can we make the product mole fractions $\alpha_1, \ldots, \alpha_n$ variables?
- Could we model it differently?

Formulating "Straightforward" Models for LP

Example: CSTR Reactor



Material Balances:

$$F_{\Delta} = \alpha_{\Delta} F_{\rm f}$$

$$F_{\rm B} = \alpha_{\rm B} F_{\rm f}$$

$$F_{C} = \alpha_{C} F_{f}$$

$$F_D = \alpha_D F_f$$

$\bullet \ \mbox{ Reaction system: } \left\{ \begin{array}{l} A+B \to C \\ B+C \to D \end{array} \right.$

• Feed flow rate: $F_{\rm f}$

• Product flow rates: F_A , F_B , F_C , F_D

Remarks:

- The α 's are for specific reactions, reactor temperature, level, mixing pattern, etc.
- If A, B, C, D are the only components,

$$\alpha_{\mathsf{A}} + \alpha_{\mathsf{B}} + \alpha_{\mathsf{C}} + \alpha_{\mathsf{D}} = 1$$

• The F's are mass units!

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Base-Delta I P Models

• Goal: Extend "straightforward" LP models to include nonlinear, secondary decision variables:

$$\mathbf{0} = \mathbf{f}(\mathbf{x},\mathbf{y}) \approx \mathbf{f}(\mathbf{x},\mathbf{y}^\circ) + \left. \frac{\partial \mathbf{f}}{\partial \mathbf{y}} \right|_{\mathbf{x}^\circ,\mathbf{y}^\circ} (\mathbf{y} - \mathbf{y}^\circ)^\mathsf{T}$$

- ▶ The base model, $f(x, y^\circ)$, describes the (linear) effect of the primary decision variables, while the secondary variables are kept constant at their nominal value $\mathbf{v} = \mathbf{v}^{\circ}$
- ► The delta model provides small corrections for deviations ("deltas") in the secondary variables y around (x°, y°)
- The accuracy of the solution depends on how well the approximation applies at $(\mathbf{x}^*, \mathbf{y}^*) \neq (\mathbf{x}^\circ, \mathbf{y}^\circ)$
- To improve the accuracy, the primary and secondary decision variables should be limited by upper and lower bounds

Approximate Models for LP

Besides "straightforward" LP models, certain classes of nonlinear or multiobjective optimization problems can be reformulated or **approximated** as LP models:

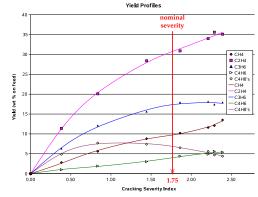
- Base-Delta Models
- Separable Programming
- Minimax and Maximin (Linear) Objectives
- Goal Programming

These approaches are usually reasonable when the uncertainties in the problem do not justify further model accuracy — Otherwise, solve the nonlinear model using NLP!

Formulating Base-Delta LP Models

Class Exercise: Pyrolysis of n-heptane





- 1 Develop a "straightforward" model that predicts the flow rate of methane from the reactor
- 2 Enhance this model by adding a delta due to changes in severity. Recommend the allowable range for the severity variable
- Is the material balance closed in the base-delta approach?

Separable Programming

• Consider the following mathematical program:

$$\min_{\mathbf{x}} \quad z \stackrel{\Delta}{=} \sum_{j=1}^{n} f_j(x_j) = f_1(x_1) + \dots + f_n(x_n)$$
s.t.
$$\sum_{j=1}^{n} a_{ij} x_j \le b_i, \quad i = 1, \dots, m$$

$$x_j \ge 0, \quad j = 1, \dots, n$$

- ► The objective consists of n nonlinear, separable terms $f_j(x_j)$, each a function of a single variable only **Examples?**
- ▶ The *m* constraints are linear
- When each f_j is convex on the feasible region, the separable program can be approximated with an LP
- An analogous situation exists when the objective is to maximize a separable concave function — Why?

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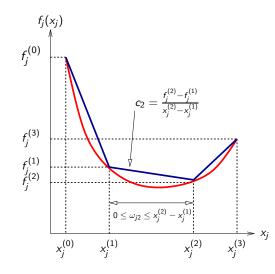
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Approximating Separable Programs as LPs

Piecewise affine approximation:

 $(N_j \text{ intervals})$



Define:

$$c_j^{(k)} = \frac{f_j^{(k)} - f_j^{(k-1)}}{x_j^{(k)} - x_j^{(k-1)}}$$
$$0 \le \omega_{jk} \le x_j^{(k)} - x_j^{(k-1)}$$

 Substitute each variable x_j and function f_j by:

$$x_j \leftarrow x_j^{(0)} + \sum_{k=1}^{N_j} \omega_{jk}$$
$$f_j(x_j) \leftarrow f_j^{(0)} + \sum_{k=1}^{N_j} c_j^{(k)} \omega_{jk}$$

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Approximating Separable Programs as LPs (cont'd)

Approximate Linear Program (on N_i Intervals):

$$\min_{\boldsymbol{\omega}} \quad \sum_{j=1}^{n} f_{j}^{(0)} + \sum_{j=1}^{n} \sum_{k=1}^{N_{j}} c_{j}^{(k)} \omega_{jk}
\text{s.t.} \quad \sum_{j=1}^{n} \sum_{k=1}^{N_{j}} a_{ij} \omega_{jk} \leq b_{i} - \sum_{j=1}^{n} a_{ij} x_{j}^{(0)}, \quad i = 1, \dots, m
0 \leq \omega_{jk} \leq x_{j}^{(k)} - x_{j}^{(k-1)}, \quad j = 1, \dots, n, \ k = 1, \dots, N_{j}$$

Important Remarks:

- Convexity guarantees that the pieces in the solutions will be included in the right order — This approach does not work if not all functions are convex!
- The solution can be made as accurate as desired by using enough intervals — One pays the price in terms of increased problem size!

Minimax and Maximin Problems

• Consider the case of multiple, competing *linear* objectives:

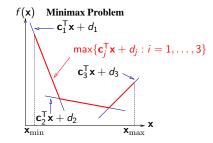
$$f_1(\mathbf{x}) \stackrel{\Delta}{=} \mathbf{c}_1^\mathsf{T} \mathbf{x} + d_1, \quad \dots, \quad f_N(\mathbf{x}) \stackrel{\Delta}{=} \mathbf{c}_N^\mathsf{T} \mathbf{x} + d_N$$

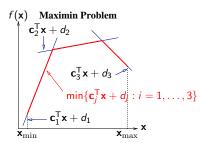
• Minimax problem: minimize the worst (greatest) objective:

$$\min_{\mathbf{x}} \max \{\mathbf{c}_i^\mathsf{T} \mathbf{x} + d_i : i = 1, \dots, N\}$$

Maximin problem: maximize the worst (least) objective:

$$\max_{\mathbf{x}} \min \{ \mathbf{c}_i^\mathsf{T} \mathbf{x} + d_i : i = 1, \dots, N \}$$





Formulating Minimax Problems

Class Exercise: Two groups of employees in a company are asked to work on Sundays, depending on the actual plant production x,

Group 1:
$$f_1(x) = 5x$$
 Group 2: $f_2(x) = 3x + 2$

The CEO wants to minimize the maximum number of employees working on Sundays in all groups. Formulate a model for this optimization problem.

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Reformulating Minimax and Maximin Problems

• Idea: Introduce a slack variable, along with N inequality constraints

Minimax Problem:

Maximin Problem:

LP Model:

$$\min_{\mathbf{x}} \max \{ \mathbf{c}_{i}^{\mathsf{T}} \mathbf{x} + d_{i} : i = 1, \dots, N \} \quad \max_{\mathbf{x}} \min \{ \mathbf{c}_{i}^{\mathsf{T}} \mathbf{x} + d_{i} : i = 1, \dots, N \}$$

LP Model:

$$\begin{array}{lll}
\min & z & \max & z \\
\text{s.t.} & z \ge \mathbf{c}_1^\mathsf{T} \mathbf{x} + d_1 & \text{s.t.} & z \le \mathbf{c}_1^\mathsf{T} \mathbf{x} + d_1 \\
& \vdots & & \vdots \\
& z > \mathbf{c}_N^\mathsf{T} \mathbf{x} + d_N & z < \mathbf{c}_N^\mathsf{T} \mathbf{x} + d_N
\end{array}$$

Additional linear constraints can be included in the formulations

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Goal Programming

• Consider the case of multiple, competing *linear* objectives:

$$f_1(\mathbf{x}) \stackrel{\Delta}{=} \mathbf{c}_1^\mathsf{T} \mathbf{x}, \quad \dots, \quad f_N(\mathbf{x}) \stackrel{\Delta}{=} \mathbf{c}_N^\mathsf{T} \mathbf{x},$$

and corresponding target levels ℓ_1, \ldots, ℓ_N

- Find a compromise between the various goals in such a way that most are to some extent satisfied
 - **Lower One-Sided Goal:** Achieve a value of at least ℓ_k for the kth goal,

$$f_k(\mathbf{x}) = \mathbf{c}_k^\mathsf{T} \mathbf{x} \ge \ell_k$$

▶ Upper One-Sided Goal: Achieve a value of at most ℓ_k for the kth goal,

$$f_k(\mathbf{x}) = \mathbf{c}_k^\mathsf{T} \mathbf{x} \leq \ell_k$$

▶ Two-Sided Goal: Achieve a value of exactly ℓ_k for the kth goal,

$$f_k(\mathbf{x}) = \mathbf{c}_k^\mathsf{T} \mathbf{x} = \ell_k$$

Formulating Goal Programming as LP Models

Soft Constraints

Target levels specify requirements that are desirable to satisfy, but which may be violated in feasible solutions

- Idea: Introduce deficiency variables, d_k^{\pm} , representing the amount by which the kth goal is over- or under-achieved
 - ▶ Lower One-Sided Goal: $\mathbf{c}_{k}^{\mathsf{T}}\mathbf{x} + d_{k}^{\mathsf{-}} = \ell_{k}, \quad d_{k}^{\mathsf{-}} \geq 0$
 - ▶ Upper One-Sided Goal: $\mathbf{c}_{k}^{\mathsf{T}}\mathbf{x} d_{k}^{+} = \ell_{k}, \quad d_{k}^{+} \geq 0$
 - ► Two-Sided Goal: $\mathbf{c}_{k}^{\mathsf{T}}\mathbf{x} + d_{k}^{\mathsf{T}} d_{k}^{\mathsf{T}} = \ell_{k}, \quad d_{k}^{\mathsf{T}}, d_{k}^{\mathsf{T}} \geq 0$
- Fundamental balances (such as material and energy balances) should never be softened! These must always be strictly observed
- Softening constraints may help debugging models in case infeasibility is reported

Formulating Goal Programming as LP Models (cont'd)

• Non-Preemptive LP Model Formulation: All the goals are considered simultaneously in the objective function,

$$\begin{aligned} & \min_{\mathbf{x}, \mathbf{d}^{\pm}} & \boldsymbol{\omega}^{\mathsf{T}} \mathbf{d}^{\pm} \\ & \text{s.t.} & \mathbf{c}_{k}^{\mathsf{T}} \mathbf{x} \pm d_{k}^{\mp} = \ell_{k}, \quad k = 1, \dots, N \\ & \quad \mathbf{A} \mathbf{x} \leq \mathbf{b} \\ & \quad \mathbf{x} \geq \mathbf{0}, \quad \mathbf{d}^{\pm} \geq \mathbf{0} \end{aligned}$$

Determining the weights ω is a subjective step... Different weights often yield very different solutions!

- <u>Preemptive</u> LP Model Formulation: The goals are subdivided into sets, and each set is given a priority
 - ► The solution proceeds by solving a sequence of subproblems, from highest to lowest priority goals
 - ▶ Goals of *lower* priority are ignored in a given subproblem
 - ► Goals of *higher* priority are enforced as hard equality constraints

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