Economics & Planning – Optimization

Chapters 12 & 14

Economics & Planning

- What ***should*** be done rather than what ***can*** be done
- Optimization
  - Combines models to…
    - Describe operations
    - Constraints to operations
  - Economics added to define costs & benefits to all actions
  - "Optimal" is best of the "feasible" possibilities
- Optimization models tend to be data-driven rather than mathematical model driven.

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Economics & Planning Applications

- Crude oil evaluation
  - Incremental value of an opportunity crude compared to base slate
  - Take into account change in products produced
- Production planning
- Day-to-day operations optimization
- Product blending & pricing
  - May have opportunity to separately purchase blend stocks
- Shutdown planning
  - Multi time periods, must take into account changes in inventories
- Multirefining supply & distribution
- Yearly budgeting
- Investment studies
- Environmental studies
- Technology evaluation

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Optimization Example

- Brewery receives order for 100 gal of 4% beer. Only have in stock 4.5% & 3.7% beers (beers A & B). Will make order by mixing these two beers and water at ***minimum ingredient cost***.

- Values:

Beer A	$0.32 per gallon
Beer B	$0.25 per gallon
Water	No cost

- Constraints:

  At least 10 gal Beer A

- Many possible solutions:

A	88.9	gallons
B	0	gallons
Water	11.1	gallons
Cost	$28.44	

- Optimal solution:

A	37.5	gallons
B	62.5	gallons
Water	0	gallons
Cost	$27.63	

Microsoft Excel Worksheet

Microsoft Word Document

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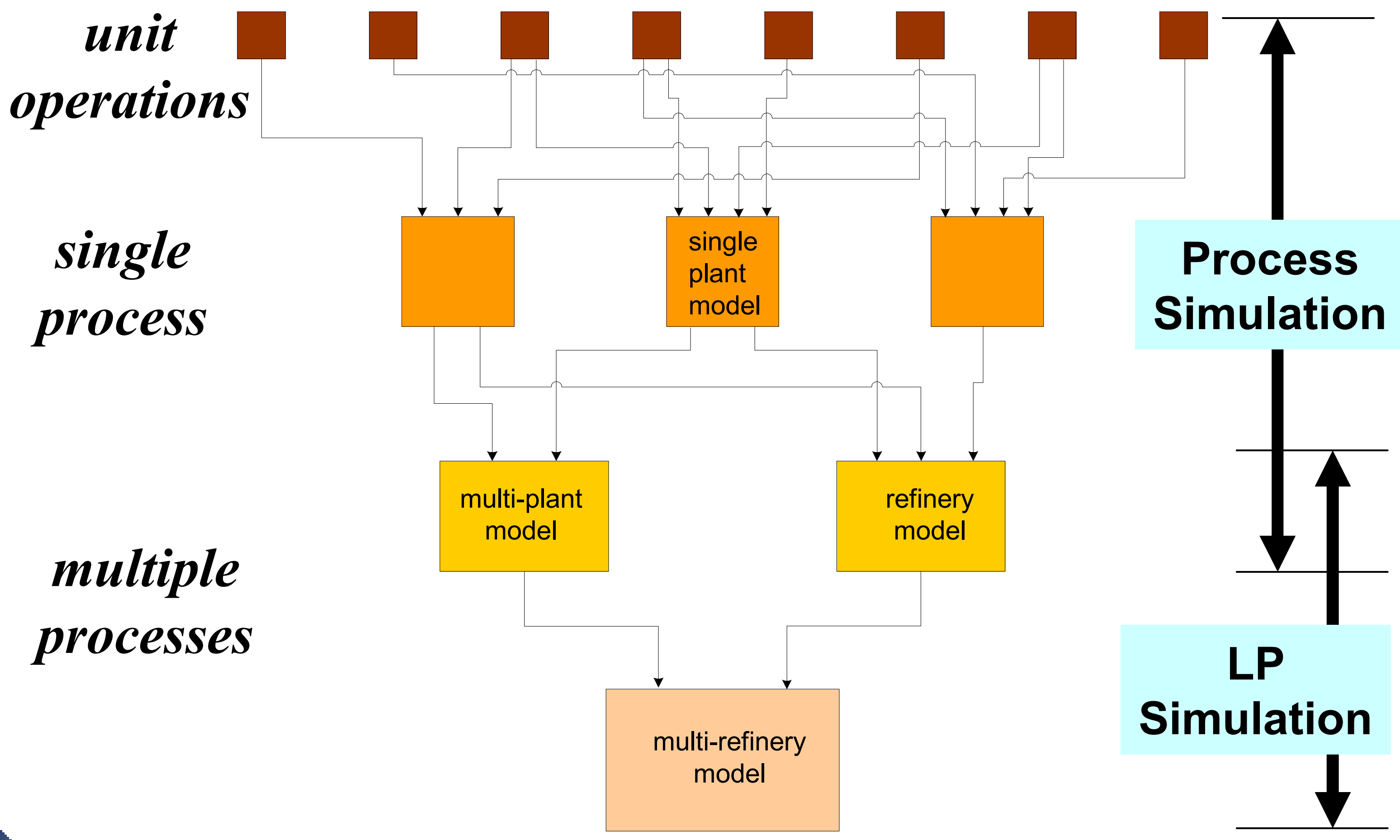
Modeling Hierarchy



Unit Representations

- Simple vector model

		Yield Vector
Feedstock		
	Butylene	-1.0000
	Isobutane	-1.2000
Product		
	n-Butane	0.1271
	Pentane	0.0680
	Alkylate	1.5110
	"Alky Bottoms	0.1190
	Tar	0.0096
Utilities		
	Steam, lb	7.28
	Power, kWh	2.45
	Cooling Water, M gal	2.48
	Fuel, MMBtu	0.69

  - For every unit of Butylene consumed, must also consume the relative amount of Isobutane, produce the shown amounts of products, & use the shown amounts of utilities

- Delta-Base model

	Feed	Base Yield	Delta K_W	Delta API
Feed	1.0	-1.0		
Hydrogen		-1500		
C5-180		8.1	1.0	3.6
180-400		28.0	-5.5	11.0
Kw	-12.1	10.9	1.2	
API	-22.0	20.0		4.0
Relative Activity	1	1	1	0.5

  - Relative activities calculated from actual properties – the Kw & API rows are zero
  - Correct base yields to take into account actual properties & relative activities

$$\text{API} = -\frac{1\times(-22.0)+1\times 20.0}{4.0} = 0.5$$

$$\text{C5-180} = \frac{1\times 8.1+1\times 1.0+0.5\times 3.6}{1} = 10.9$$

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What is “Linear Programming”?

- Word “Programming” used here in the sense of “planning”
- For N independent variables ***maximize***

$$z = a_{01}x_1 + a_{02}x_2 + \cdots + a_{0N}x_N$$

- Subject to the primary constraints

$$x_1 \geq 0, x_2 \geq 0, \ldots, x_N \geq 0,$$

- and to M additional constraints (all b_n positive)

$$a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{iN}x_N \leq b_i$$
$$a_{j1}x_1 + a_{j2}x_2 + \cdots + a_{jN}x_N \geq b_j$$
$$a_{k1}x_1 + a_{k2}x_2 + \cdots + a_{kN}x_N = b_k$$

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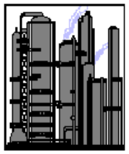
Linear Programming

- From *Numerical Recipes in Fortran 77, The Art of Scientific Computing*, by Press, Teukolsky, Vetterling, & Flannery:

  "… the subject of linear programming is surrounded by notational and terminological thickets. Both of these thorny defenses are lovingly cultivated by a coterie of stern acolytes who have devoted themselves to the field. Actually, the basic ideas of linear programming are quite simple. Avoiding the shrubbery, we want to teach you the basics by means of a couple of specific examples; it should then be quite obvious how to generalize."



Linear Programming Terminology

- Objective Function
  - Function z to be maximized
- Feasible Vector
  - A set of values $x_1, x_2, \ldots, x_N$ that satisfies all constraints
- Optimal Feasible Vector
  - Feasible vector that maximizes the objective function

Linear Programming Problem Solutions

- Solutions will tend to be in the "corners" of where the constraints meet
- May have an infinite number of solutions along a constraint edge
- May not have a solution
  - Incompatible constraints
  - Feasible area unbounded towards the maximum

Sample 2D LP Problem

- Objective function

$$\text{Maximize}\ \ z = x_1 - 3x_2$$

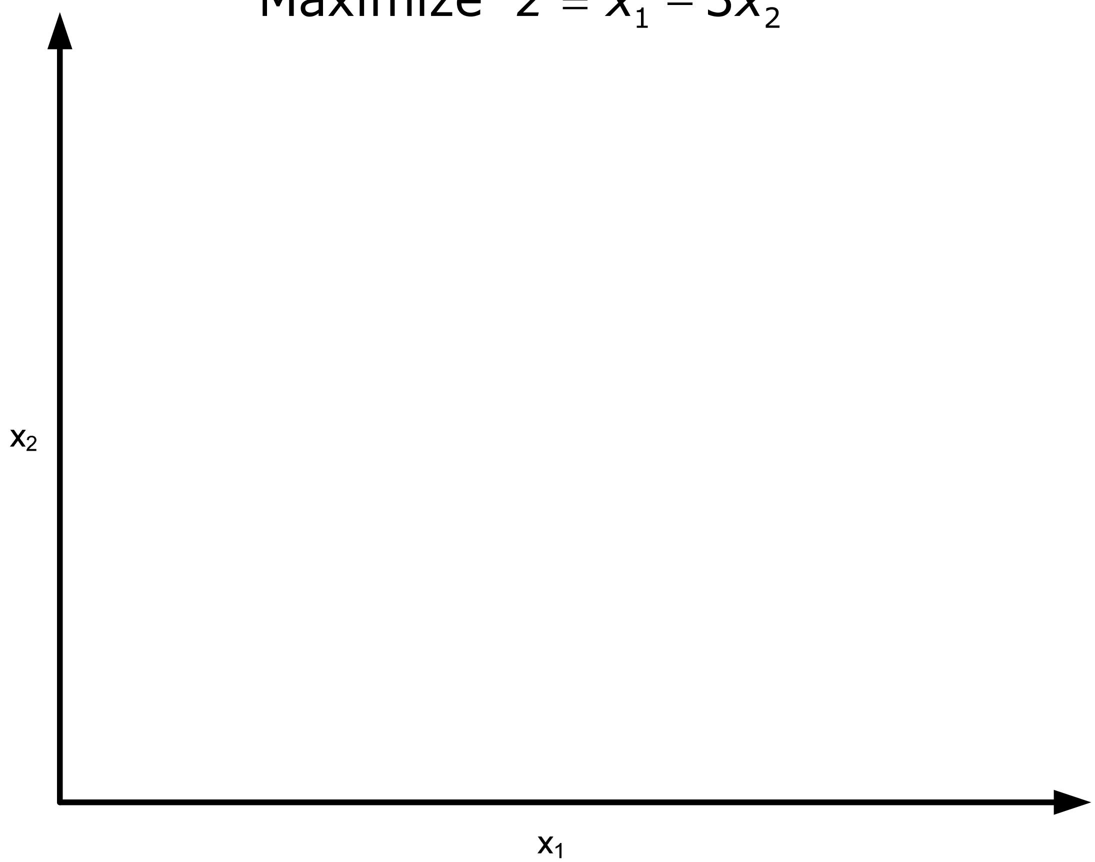
- Constraints

$$\begin{aligned} -2x_1 + x_2 &\le 4 \\ 0.5x_1 + x_2 &\le 20 \\ 1.5x_1 - x_2 &\le 10 \\ 3x_1 + x_2 &\le 30 \end{aligned}$$

Sample 2D LP Problem

Maximize $z = x_1 - 3x_2$

$$-2x_1 + x_2 \leq 4$$
$$0.5x_1 + x_2 \leq 20$$
$$1.5x_1 - x_2 \leq 10$$
$$3x_1 + x_2 \leq 30$$



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Sample 2D LP Problem

Maximize $z = x_1 - 3x_2$

$-2x_1 + x_2 \leq 4$

$0.5x_1 + x_2 \leq 20$

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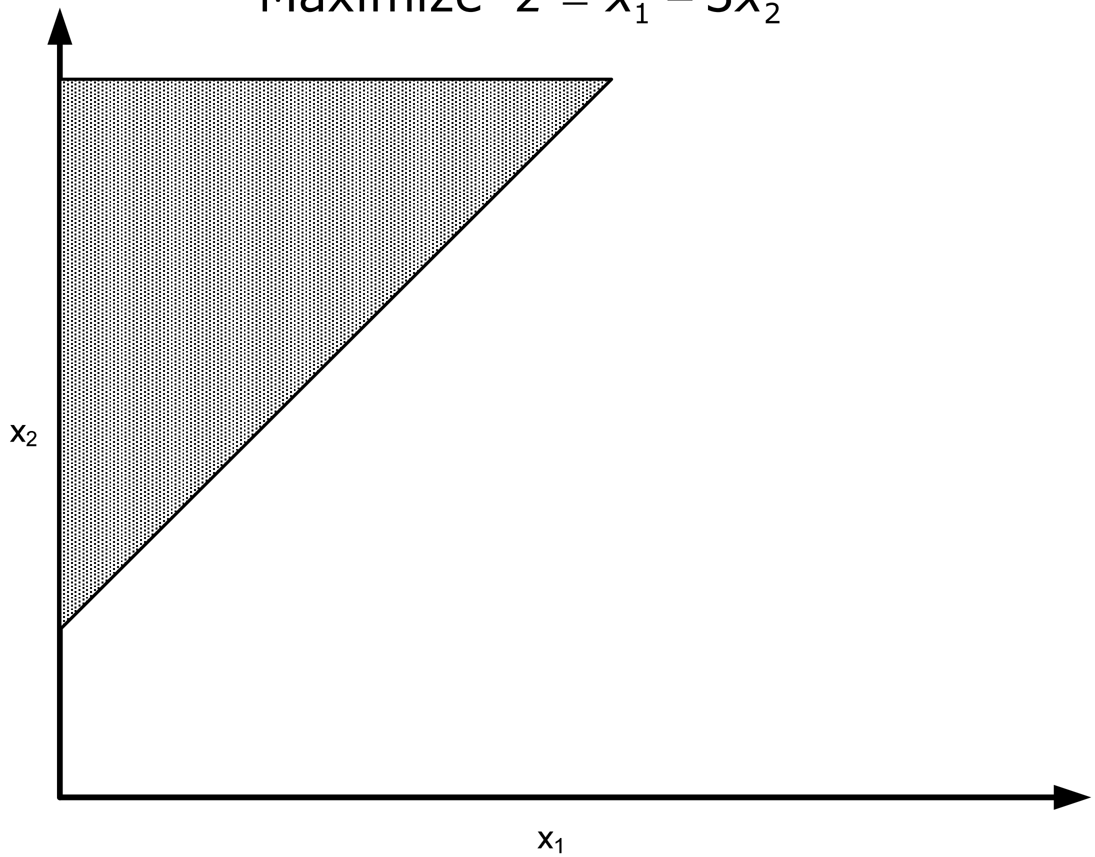

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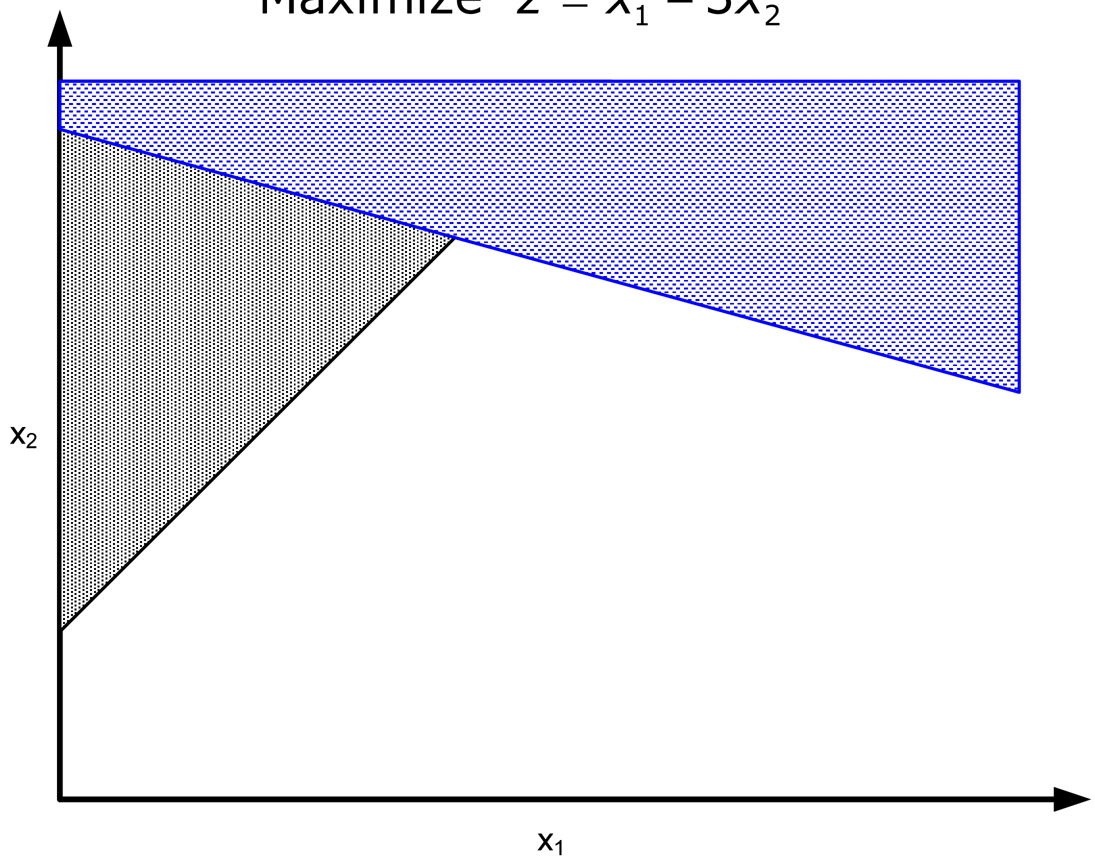

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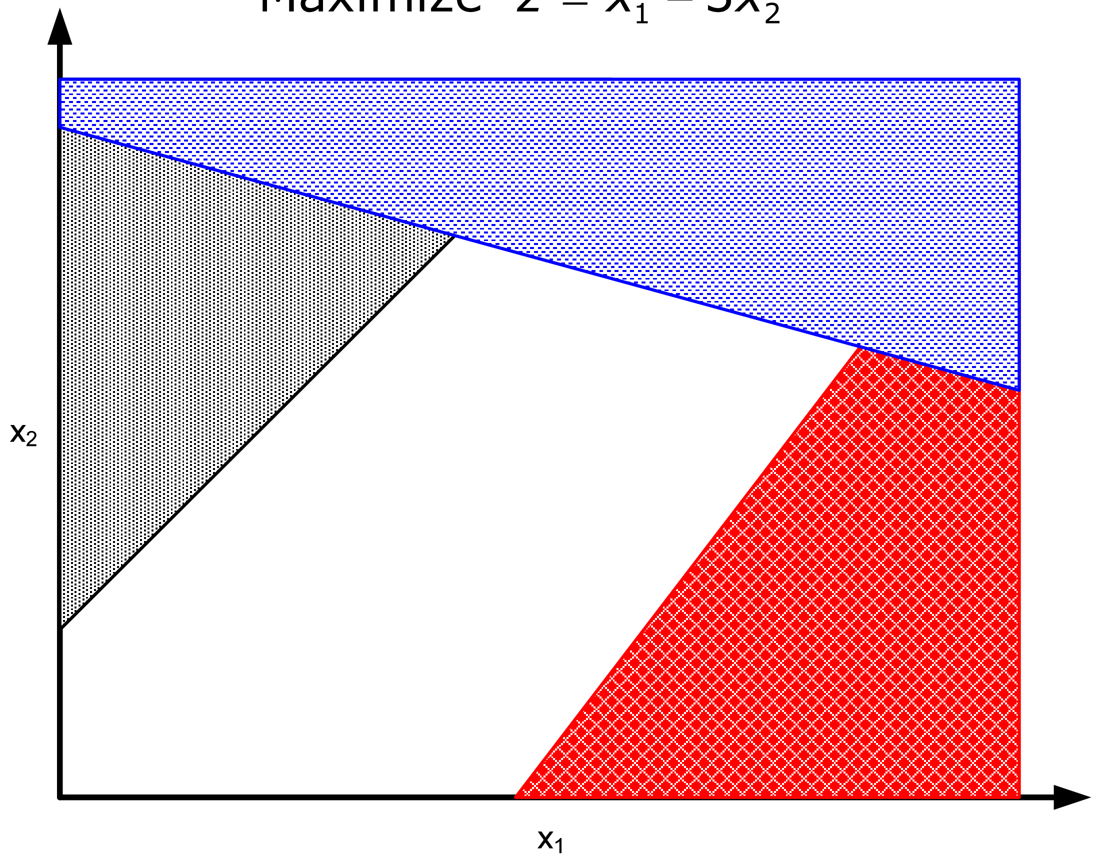

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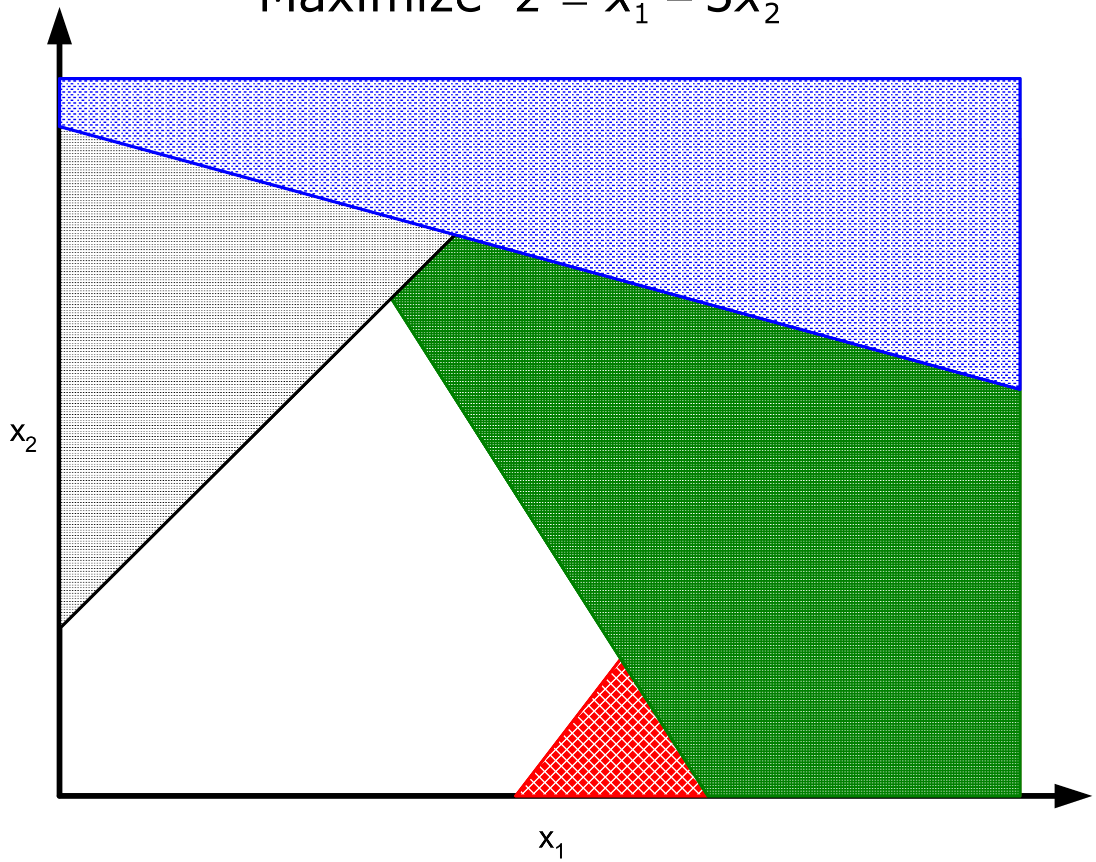

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Sample 2D LP Problem

Maximize $z = x_1 - 3x_2$

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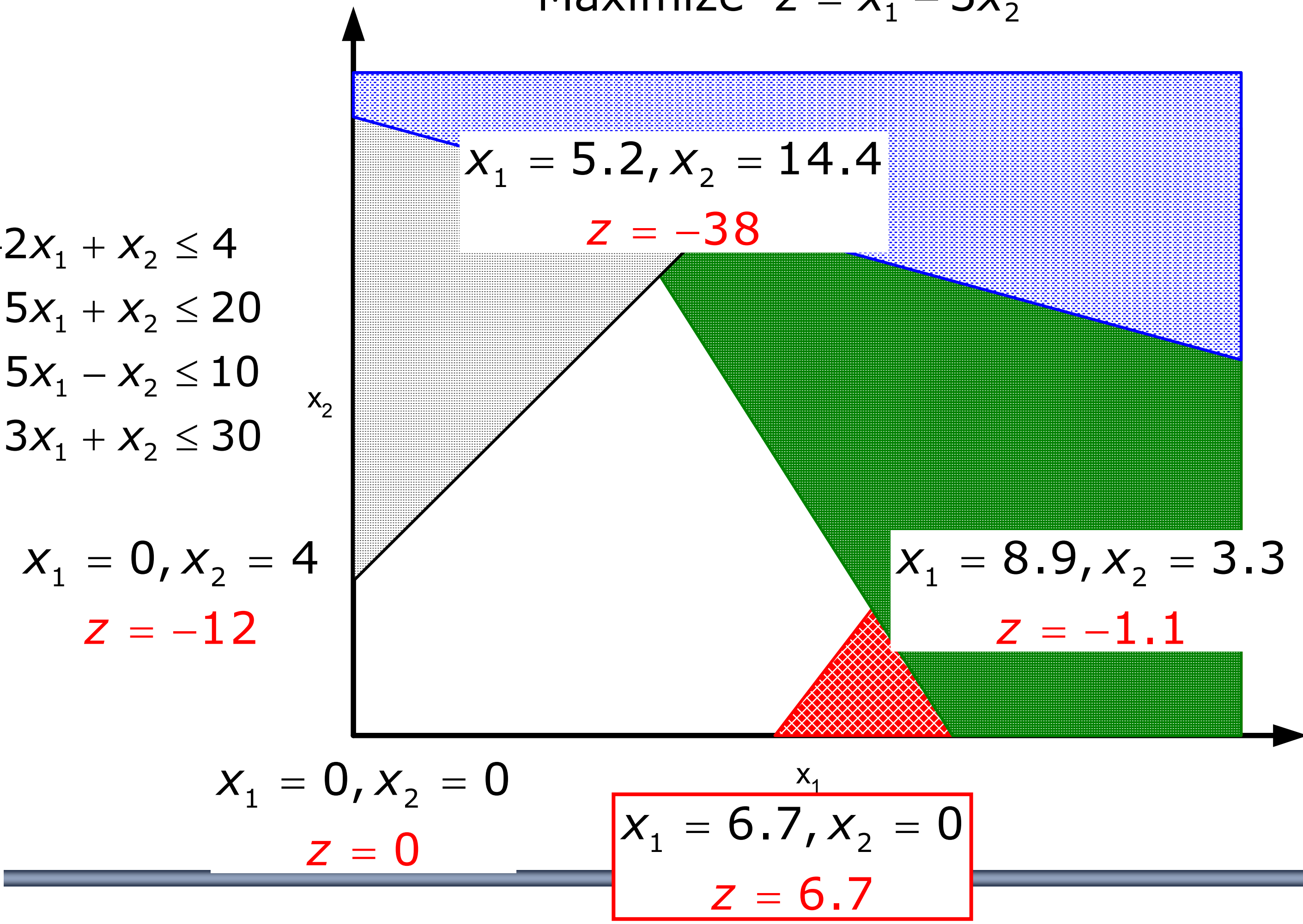

Simplex Method

- First published by Danzig in 1948
- Organized procedure to go from "corner" to "corner" & find the optimal solution vector
- Introduce "slack variables" to make all inequality constraints equality constraints
  - Slack variable equal to zero means constraint is active
  - Example:

$$-2x_1 + x_2 \leq 4 \quad \Rightarrow \quad -2x_1 + x_2 + y_1 = 4 \text{ where } y_1 \geq 0$$

- Need to re-organize problem into a "restricted normal form" and examine all of the coefficients in a "tableau"

Tableau Rows & Columns

- Rows are *constraints*
  - Represent limits of operation
  - Only enter optimal solution if actually limiting
  - Material balances, utility balances, unit capacities, etc.
- Columns are *variables*
  - An LP has more columns than rows
  - ***Column Activity*** — value of variable
  - Columns generally represent flows in the process
  - Solution vector — column activities which maximize or minimize objective function

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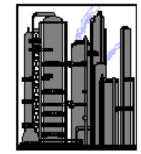
LP Software



- Advantages of specialty software
  - Creates the coefficients in the tableau
  - Solves the LP problem
  - Creates a report with interpreted values

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Problems with LPs

- Nonlinear blending
  - Linearize with blending factors

$$(\text{RVP})^{1.25} = \sum v_i (\text{RVP})_i^{1.25}$$

  - Modify form of "ratio" models

$$\gamma_o = \sum v_i \gamma_{o,i} = \frac{\sum V_i \gamma_{o,i}}{\sum V_i} \Rightarrow \gamma_o \sum V_i = \sum V_i \gamma_{o,i}$$

$$0 = \sum V_i \left(\gamma_{o,i} - \gamma_o \right)$$

- Stream pooling problem
- Nonlinear responses of processes to changes in feedstock quality or operating conditions
- Aggregation/segregation of feedstocks
- Accuracy of solution away from baseline

Non-Linear Programming

- Can more closely match the physics of the problem
  - Example: octane blending models

$$R = \bar{R} + 0.03324\left[\overline{RJ} - \bar{R}\cdot\bar{J}\right] + 0.00085\left[\overline{\left(O^2\right)} - \bar{O}^2\right]$$

$$M = \bar{M} + 0.04285\left[\overline{MJ} - \bar{M}\cdot\bar{J}\right] + 0.00066\left[\overline{\left(O^2\right)} - \bar{O}^2\right] - 6.32\times10^{-7}\left[\overline{\left(A^2\right)} - \bar{A}^2\right]$$

- Guarantees of solutions are more tenuous
  - Not necessarily at constraints
  - Discontinuous feasible regions possible
- Types of optimization algorithms
  - Local optimization
    - Based on following gradients
      - Excel's Solver based on GRG2
  - Global optimization
    - Randomly search overall region before switching to local optimization technique
      - Simulated annealing

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Product Blending Example

Raw Materials

Properties for Blending Calculations

	RON	MON	RVP	Aromatics	Olefins
Butane	93.8	89.6	52	0.0	0.0
Straight Run Naphtha	63.7	61.2	10.8	2.2	0.9
Isomerate	78.6	80.5	8	1.6	0.1
Reformate (Low Octane)	97.3	86.7	3.2	61.1	1.0
Reformate (High Octane)	109.3	100.4	1	94.2	0.6
FCC Naphtha	93.2	81	4.3	35.2	32.6
Alkylate	93.2	91.2	4.6	0.5	0.2

	Cost & Availability			*Usage*		
	Cost ($/gal)	Minimum Required	Maximum Available	Regular	Premium	Total
Butane	**1.20**		**25,000**			0
Straight Run Naphtha	**1.20**		**50,000**			0
Isomerate	**1.80**		**0**			0
Reformate (Low Octane)	**1.90**		**0**			0
Reformate (High Octane)	**2.40**		**35,000**			0
FCC Naphtha	**1.90**		**50,000**			0
Alkylate	**2.00**		**12,000**			0

Products

	Lower & Upper Limits on Properties		*Price & Production Requirements*		
	Octane Number	RVP	Price ($/gal)	Minimum Required	Maximum Allowed
Regular	**89**	**9.0**	**2.20**	**75,000**	
Premium	**92**	**9.0**	**2.40**		**40,000**

Product Blending Example

Raw Materials

	Properties for Blending Calculations						
	RON	MON	(R+M)/2	RVP	$RVP^{1.25}$	Aromatics	Olefins
Butane	93.8	89.6	91.7	52	139.6	0.0	0.0
Straight Run Naphtha	63.7	61.2	62.45	10.8	19.6	2.2	0.9
Isomerate	78.6	80.5	79.55	8	13.5	1.6	0.1
Reformate (Low Octane)	97.3	86.7	92	3.2	4.3	61.1	1.0
Reformate (High Octane)	109.3	100.4	104.85	1	1.0	94.2	0.6
FCC Naphtha	93.2	81	87.1	4.3	6.2	35.2	32.6
Alkylate	93.2	91.2	92.2	4.6	6.7	0.5	0.2

	Cost & Availability			*Usage*				
	Cost ($/gal)	Minimum Required	Maximum Available	Regular	Premium	Total	Minimum Slack	Maximum Slack
Butane	**1.20**	**0**	**25,000**	**0**	**0**	0	**0**	**25,000**
Straight Run Naphtha	**1.20**	**0**	**50,000**	**0**	**0**	0	**0**	**50,000**
Isomerate	**1.80**	**0**	**0**	**0**	**0**	0	**0**	**0**
Reformate (Low Octane)	**1.90**	**0**	**0**	**0**	**0**	0	**0**	**0**
Reformate (High Octane)	**2.40**	**0**	**35,000**	**0**	**0**	0	**0**	**35,000**
FCC Naphtha	**1.90**	**0**	**50,000**	**0**	**0**	0	**0**	**50,000**
Alkylate	**2.00**	**0**	**12,000**	**0**	**0**	0	**0**	**12,000**

Products

	Lower & Upper Limits on Properties						*Price & Production Requirements*		
	Octane Number		RVP		$RVP^{1.25}$		Price ($/gal)	Minimum Required	Maximum Allowed
Regular	**89**	**110**	**0.0**	**9.0**	0.0	15.6	**2.20**	**75,000**	**1,000,000**
Premium	**92**	**110**	**0.0**	**9.0**	0.0	15.6	**2.40**	**1**	**40,000**

Product Calculations

	Volumes & Properties						*Cost & Revenue*		
	Produced	RON	MON	(R+M)/2	RVP	$RVP^{1.25}$	Revenue ($)	Cost($)	Profit ($)
Regular	0	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	$0	$0	$0
Premium	0	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	$0	$0	$0
Total	0						$0	$0	**$0**

Product Constraints

	Lower Limit			*Upper Limit*	
	Value	Slack	*Actual*	Value	Slack
Volume Regular	75,000	**-75,000**	0	1,000,000	**1,000,000**
Octane Regular	89.0	**#DIV/0!**	#DIV/0!	110.0	**#DIV/0!**
RVP Regular	0.0	**#DIV/0!**	#DIV/0!	9.0	**#DIV/0!**
Volume Premium	1	**-1**	0	40,000	**40,000**
Octane Premium	92.0	**#DIV/0!**	#DIV/0!	110.0	**#DIV/0!**
RVP Premium	0.0	**#DIV/0!**	#DIV/0!	9.0	**#DIV/0!**

Product Blending Example

Raw Materials

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Alkylate	93.2	91.2	92.2	4.6	6.7	0.5	0.2

	Cost & Availability			*Usage*				
	Cost ($/gal)	Minimum Required	Maximum Available	Regular	Premium	Total	Minimum Slack	Maximum Slack
Butane	**1.20**	**0**	**25,000**	**5,385**	**2,890**	8,274	**8,274**	**16,726**
Straight Run Naphtha	**1.20**	**0**	**50,000**	**10,610**	**4,474**	15,084	**15,084**	**34,916**
Isomerate	**1.80**	**0**	**0**	**0**	**0**	0	**0**	**0**
Reformate (Low Octane)	**1.90**	**0**	**0**	**0**	**0**	0	**0**	**0**
Reformate (High Octane)	**2.40**	**0**	**35,000**	**20,755**	**14,245**	35,000	**35,000**	**0**
FCC Naphtha	**1.90**	**0**	**50,000**	**39,482**	**10,518**	50,000	**50,000**	**0**
Alkylate	**2.00**	**0**	**12,000**	**4,127**	**7,873**	12,000	**12,000**	**0**

Products

	Lower & Upper Limits on Properties						*Price & Production Requirements*		
	Octane Number		RVP		$RVP^{1.25}$		Price ($/gal)	Minimum Required	Maximum Allowed
Regular	**89**	**110**	**0.0**	**9.0**	0.0	15.6	**2.20**	**75,000**	**1,000,000**
Premium	**92**	**110**	**0.0**	**9.0**	0.0	15.6	**2.40**	**1**	**40,000**

Product Calculations

	Volumes & Properties						*Cost & Revenue*		
	Produced	RON	MON	(R+M)/2	RVP	$RVP^{1.25}$	Revenue ($)	Cost($)	Profit ($)
Regular	80359	93.5	84.5	89.0	9.0	15.59	$176,790	$152,276	$24,514
Premium	40000	95.7	88.3	92.0	9.0	15.59	$96,000	$78,755	$17,245
Total	120359						$272,790	$231,031	**$41,759**

Product Constraints

	Lower Limit		*Actual*	*Upper Limit*	
	Value	Slack		Value	Slack
Volume Regular	75,000	**5,359**	80,359	1,000,000	**919,641**
Octane Regular	89.0	**0.0**	89.0	110.0	**21.0**
RVP Regular	0.0	**9.0**	9.0	9.0	**0.0**
Volume Premium	1	**39,999**	40,000	40,000	**0**
Octane Premium	92.0	**0.0**	92.0	110.0	**18.0**
RVP Premium	0.0	**9.0**	9.0	9.0	**0.0**