8. Problem Formulation

In this section you will learn the following concepts:

1. Defining decision variables
    a. Independent versus dependent
    b. Discrete versus continuous
2. Defining variable bounds
3. Defining types of constraints
    a. Inequality versus equality
    b. Independence of inequality direction
4. Defining an objective function
5. Feasible regions
    a. Defining boundaries
    b. Plotting and visualizing feasible regions
    c. Feasible search directions
    d. Improving search directions
    e. Examples of graphical solutions
6. Scenarios of optimal outcomes

8.1. The Importance of a Good Formulation

In this course, we have explored how to develop Net Value Functions (NVFs) to help us make engineering decisions. Now, we turn our attention to how to optimize NVFs given a set of parameters and constraints. Before we dive into optimization, it is important to lay the groundwork by properly formulating our model. Note: NVFs are mathematical models developed based on the problems/scenarios we have. We will use the term models throughout this lecture note.

In model-based optimization, conclusions are drawn from the *model* of the system, NOT from the problem itself. As a result, it is critical to **develop an appropriate model for your system/problem/scenario**. An inadequate model will lead to false conclusions, even if the solution of the model itself is "correct" according to the model equations.

All models are wrong. Some models are useful. – George Box

Moreover, it is important that the model is **computationally tractable** for it to be practical. Enormous models with very high levels of detail and thousands of complicated nonlinear equations may seem nice from a modeling accuracy perspective, but it will prove very difficult to solve computationally. A **trade-off** exists between model accuracy and computational efficiency (*aka* tractability).

*Think about how slow it was for Excel to generate the Monte Carlo Simulation in Week 6 and sometimes it did not complete all the runs!

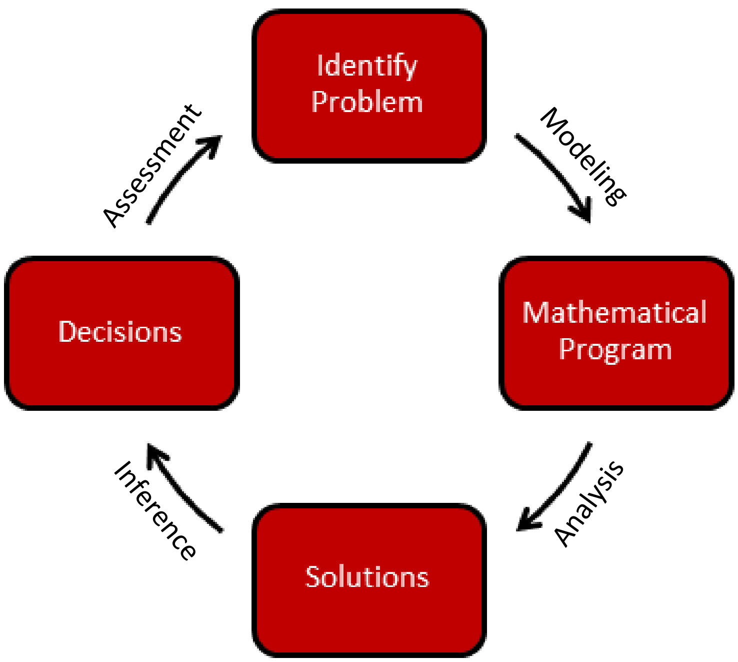
Model Validity versus Tractability

- The **VALIDITY** of a model is the degree to which inferences drawn from it hold real meaning for the system we are modeling.
- The **TRACTABILITY** of a model is the degree to which the model permits convenient analysis. This includes the ability for us (the users) to analyze results as well as the ability of the computer to generate those results.

There is always a **trade-off** between validity and tractability. We may make a "better" model, but this usually comes at the cost of additional complexity.

The model-based optimization procedure is typically *iterative* as shown in the figure below. Often, **defining the problem** is just as important as actually solving it; by defining an optimization problem, you are identifying the areas in which your system can improve.

We find it useful to formulate an optimization problem even if we cannot solve it. – Dofasco



8.2. Forming Optimization Models

In general terms, optimization models (mathematical programs) represent problem choices as *decision variables* that attempt to seek the maximum (or minimum) of an *objective function.* An objective function must be dependent on one or more decision variables. The ranges over which decision variables are permitted are typically subjected to *constraints*. In the context of this course, the objective function is our NVF, and the decision variables are the parameters we identified for the NVF.

Generalized Optimization Program

$$\min_{\boldsymbol{x}} \phi = f(\boldsymbol{x}) \qquad \leftarrow \text{Objective Function}$$

$$s.t. \qquad \leftarrow \text{“Subject to”}$$

$$h(\boldsymbol{x}) = 0 \qquad \leftarrow \text{Equality Constraints}$$

$$g(\boldsymbol{x}) \leq 0 \qquad \leftarrow \text{Inequality Constraints}$$

$$\boldsymbol{x}_{lb} \leq \boldsymbol{x} \leq \boldsymbol{x}_{ub} \qquad \leftarrow \text{Variable Bounds}$$

8.2.1. Decision Variables

Decision variables $\boldsymbol{x}$ may be grouped into one of two classes: **independent** and **dependent**. This delineation does not mean much in the long run but can be useful at the formulation stage to minimize the complexity of the problem. During the solution stage, dependent variables are usually constrained according to the model constraints and independent variables.

- **Independent Variables** can be manipulated to change the behaviour of the system. Example: hourly wage and labour hours
- **Dependent Variables** are often expressed as more “convenient” combinations of independent variables for the sake of visualization, but in practice do not have an impact on the solution. Example: Labour cost, which is the product of the independent variables: hourly wage and labour hours

Examples of Decision Variables

- Capital costs
- Operation costs
- Environmental impact
- Risk tolerance
- Maximum investment permitted
- Projected revenue
- Social impact

8.2.2. Discrete Versus Continuous Variables

A decision variable is **discrete** if it is limited to a fixed or countable set of values (all-or-nothing, either-or, must be produced/purchased in integer quantities, *etc.*). Mathematically speaking, it means a set of discrete decision variables $\boldsymbol{x}_D$ (sometimes called $\boldsymbol{y}$) takes the form:

$$\boldsymbol{x}_D \in \boldsymbol{I} = \{0, 1, 2, \ldots\}$$

A variable is **continuous** if it may take on *any value* in a specified interval. A set of continuous variables $\boldsymbol{x}_C$ is therefore defined to be:

$$\boldsymbol{x}_C \in \boldsymbol{S} \subset \mathbb{R}$$

Where that weird “⊂” means “is a subset of.”

A **heuristic** about selecting appropriate variables is that *modeling with continuous variables is preferred over modeling with discrete variables*. This is for tractability reasons (think of numerical methods – It is far easier to solve a continuous function than a discontinuous function).

Another **heuristic** regarding discrete versus continuous variables is that if a discrete variable scale is large enough so that rounding to the nearest integer is possible with *minimal loss of model accuracy*, that variable can be modeled *continuously*.

8.2.3. Indexing Variables

In real applications, optimization problems can become quite large. They can quickly grow to thousands of equations, millions of variables, and more! We clearly do not want to write them all out (no, really), so we typically exploit **indexed notational schemes** to keep large models manageable during formulation. Indexing is typically used to condense multiple dimensions of decisions into a single variable.

Indexing

Indexes (or **subscripts**) permit the representation of collections of similar pieces of information with a single symbol. For example, we might define a variable x_i which represents a decision about each value of $\boldsymbol{x}$ for, say, 100 values of index i:

$$\{x_i : i = 1 \ldots 100\}$$

The first step of defining an optimization model is to choose appropriate indexes for each dimension of the problem. **Multiple indexes** in the same problem (for the same variable) are very common.

8.2.3.1. Indexing In-Class Example

Consider the following example:

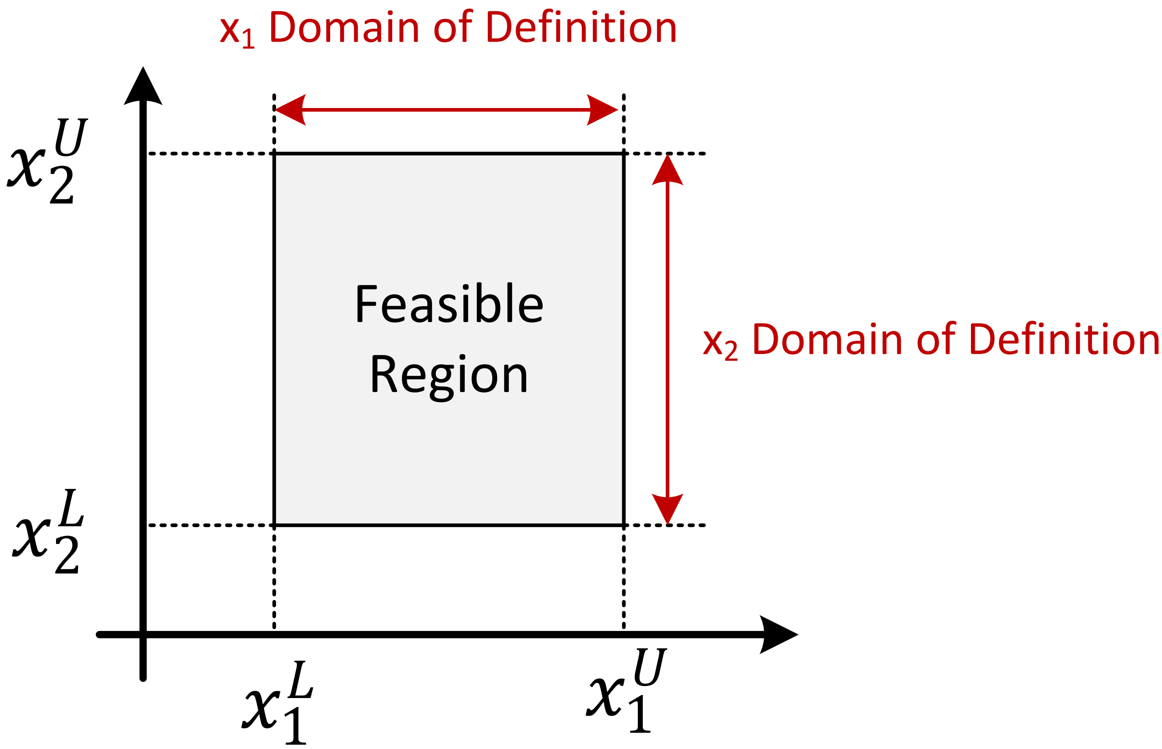
A large food manufacturer operates 20 different manufacturing plants. Each plant has the capability of producing 30 different types of pre-packaged foods and can supply 25 different customers across a given market. We may denote the dimensions of the problem as:

- p is the plant facility number: $p = \{1, \cdots, 20\}$
- f is the food product produced: $f = \{1, \cdots, 30\}$
- r is the sales region that can be supplied by a given plant: $r = \{1, \cdots, 25\}$

1. Based on this scenario, what might be the variables for this problem (in words)?
2. Using indexing, define the appropriate decision variables for this problem (mathematically)
3. What is the total number of decision variables for this model?

8.2.4. Variable Bounding

Decision variables are usually *bounded* in optimization problems to reflect physical reality (cannot purchase negative raw materials, cannot have a temperature less than 0 K) and model assumptions (cannot sleep less than 6 hours per day). The upper ($\boldsymbol{x}^U$) and lower bounds ($\boldsymbol{x}^L$) for given variables define their so-called **domain of definition**. The combination of domains of definition provides what is known as the **feasible region** or **feasible set** (more on this later).



8.2.4.1. Remarks

- Assigning the minimum and maximum values to the same number sets that variable to a specific value → $x_i^L = x_i^U = x_i$ for some i.
- The most common variable bound is **non-negativity** → $x_i \geq 0 \;\; \forall \;\; i$

Notation comment – the upside-down "A" (∀) *is the "for all" symbol.*

8.2.5. Constraints

Constraints are self-imposed or physically realizable restrictions and interactions between decision variables that further limit the allowable values of those variables. There are two types of constraints generally used in optimization: **inequality constraints** and **equality constraints**.

Inequality Constraints
Inequality constraints are defined as any constraints conforming to:

$$g(\boldsymbol{x}) \leq \boldsymbol{0}$$

- **One-Way** limits on the system and are *essential* for optimization.
- Inequality constraints of the form ≥ 0 may be re-written to appear as ≤ 0.
- There can be many of these constraints $\Rightarrow g(\boldsymbol{x})$ is a *vector* that can be **indexed**.
- Inequalities are critical to defining the bounds of a feasible region and preventing **unbounded solutions**.

There are several reasons that we might want to limit the values a given variable can take, such as:

- Safety
- Product qualities (contracts, performance)
- Equipment damage (long term, short term [failure])
- Operating windows
- Legal/ethical concerns
- Prevents regions of mathematical/physical inconsistencies

Examples of inequality constraints

- Maximum allowable investment
- Minimum voltage required
- Maximum load on a beam
- Maximum pressure in a sealed vessel
- Maximum region in which a simplification/approximation is valid

Equality Constraints
Equality constraints are defined as any constraints conforming to:

$$h(\boldsymbol{x}) = \boldsymbol{0}$$

- These describe interactions or physical relationships between variables in the model.
- Written with a **zero RHS** according to convention.
- There can be multiple equality constraints so that $h(\boldsymbol{x})$is a vector that can be **indexed**.
- There **CANNOT** be more independent equality constraints than decision variables in the model. Think back to your numerical methods class and convince yourself as to why this is true.

Examples of equality constraints

- $F = ma$
- V=IR
- $P_1V_1=P_2V_2$

8.2.6. The Objective Function

The objective function is our method to evaluate the impacts of decision variables. For the purposes of this course, the net value function is an example of an objective function.

Objective Function

The objective function ϕ is a function of the decision variables $\boldsymbol{x}$ for which we want to find the *minimum* or *maximum*. For example:

$$\min_{\boldsymbol{x}} \phi = f(\boldsymbol{x})$$

- We require the objective function to be **quantitative** (numerical), rather than qualitative.
- A scalar objective function is preferred, although many multi-objective problems exist. In these cases, it is sometimes possible to combine objectives into a single scalar quantity.
- There is no fundamental (mathematical) or practical difference between *maximization* and *minimization* problems (why?). That is: $\min_{\boldsymbol{x}} \phi_1 = f(\boldsymbol{x}) \Leftrightarrow \max_{\boldsymbol{x}} \phi_2 = -f(\boldsymbol{x})$

Examples of scalar quantities representing performance

- Maximize net value
- Maximize profit (or minimize cost)
- Maximize product quality
- Minimize energy use
- Minimize environmental footprint
- Minimize time required to complete a task
- Maximize anticipated safety (how do you get a single value for this?)

Consider a **linear** optimization problem with variables x_i each with associated costs c_i for the set $i = \{1, 2, \dots, n\}$. We can define the *objective function* for this problem in two ways.

1) We can express it as a summation of indexed variables: $\min_{x} \phi = \sum_i x_i c_i$
2) We can express it as a product of vectors: $\min_{x} \phi = c^T x$

8.2.6.1. Model Formulation Example 1 – Crude Distillation

A refinery under your supervision distills crude petroleum into **three** products: gasoline, jet fuel, and lubricants. Your plant receives crude oil shipments from **two** locations: Canada and USA. The chemical compositions of the crude from each location are slightly different, and thus yield different products per unit of crude oil refined. You may assume that the qualities from each location are constant.

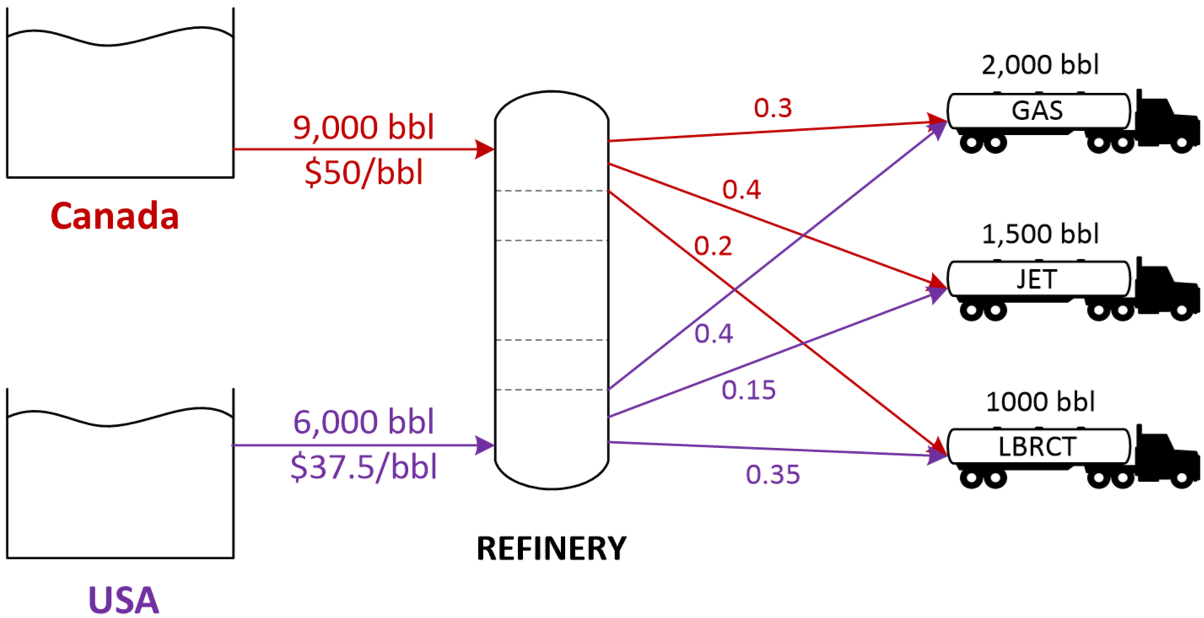
- Each barrel from Canada yields 0.3 barrels of gasoline, 0.4 barrels of jet fuel, and 0.2 barrels of lubricants.
- Each barrel from USA yields 0.4 barrels of gasoline, 0.15 barrels of jet fuel, and 0.35 barrels of lubricants.
- The remaining 0.1 (10%) from both sources is lost to the refining process.

The crudes also differ in availability and cost:

- The Canadian oil costs your refinery $50 per barrel and is available up to 9,000 barrels per day.
- The American crude costs your refinery $37.5 but only available up to 6,000 barrels per day.

You have a contract with local distributors to provide **2,000 barrels of gasoline**, **1,500 barrels of jet fuel**, and **1000 barrels of lubricants** per day.
Your task is to **draw a diagram of the supply network** and **formulate** the optimization problem for this scenario.

8.2.6.2. Model Formulation Example 1 Solution



The formulation of this problem can be written as follows (note that other formulations are possible). In the following formulation, x_1 represents the number of barrels purchased from Canada and x_2 is the number of barrels purchased from USA.

$$\min_{x_1,x_2} \phi = 50x_1 + 37.5x_2$$

Subject to

$$\begin{aligned}
0.3x_1 + 0.4x_2 &\geq 2,000 \\
0.4x_1 + 0.15x_2 &\geq 1,500 \\
0.2x_1 + 0.35x_2 &\geq 1,000 \\
x_1 &\leq 9,000 \\
x_2 &\leq 6,000 \\
x_i &\geq 0 \qquad (\forall\, i)
\end{aligned}$$

This formulation can then be translated into MATLAB, or Microsoft Excel for solving. This solution can also be done *graphically*, but we will get to that later. Do you see what the answer is before even optimizing? It might not be that obvious.

8.2.7. Graphing Model Constraints

In many small models, such as 2- or 3-dimensional models, it is useful to plot constraints and objective contours to arrive at a graphical solution. When graphing a potential optimization problem, we are faced with the requirement of forming the **feasible set**:

Feasible Set

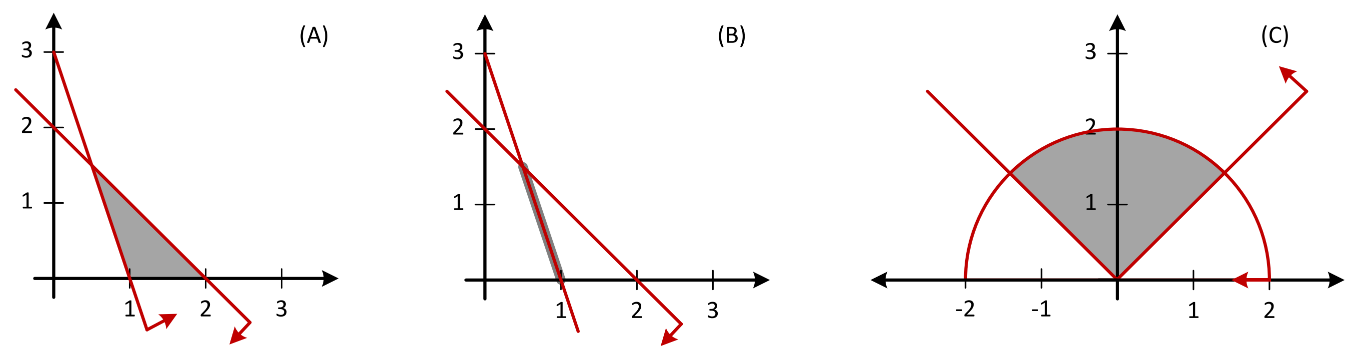
The feasible set (or region) $\mathcal{S}$ of an optimization model is the collection of decision variables that satisfy *all* the model constraints:

$$\mathcal{S} \triangleq \{\boldsymbol{x} : g(\boldsymbol{x}) \leq 0, h(\boldsymbol{x}) = 0, x^L \leq x \leq x^U\}$$

- The set of all points satisfying $h(x) = 0$ results in a **line** or **vector** when plotting the feasible set.
- The set of all points satisfying $g(x) \leq 0$ results in a **region** bounded above ($\leq$) or below ($\geq$) by a line defining the inequality.

For example, consider the following three sets of constraints, which result in the feasible regions shown in the figure below:

Constraint set (A)	*Constraint set (B)*	*Constraint set (C)*
$x_1 + x_2 \leq 2$	$x_1 + x_2 \leq 2$	$x_1^2 + x_2^2 \leq 4$
$3x_1 + x_2 \geq 3$	$3x_1 + x_2 = 3$	$\lvert x_1 \rvert - x_2 \leq 0$
$x_1, x_2 \geq 0$	$x_1, x_2 \geq 0$	



8.2.8. Graphing Objective Functions

Graphing objective functions in two dimensions requires the plotting of the objective function as **contours**. Knowing the objective function and how it behaves in the feasible region is critical to solve an optimization problem graphically.

Objective Contour

The contour C_ϕ of an objective function ϕ (in the decision variable space) is the line or curve passing through values of the decision variables $\boldsymbol{x}$ having a **constant value for the objective function** ϕ:

$$C_\phi \triangleq \{\boldsymbol{x} : f(\boldsymbol{x}) = \phi\}$$

The **easiest way to plot objective contours** is to assign a value for ϕ, treat it as a constant, and plot the resulting profile on the (x_1, x_2) axes. For example, consider the following two small, constrained optimization problems, resulting in the feasible regions and objective contours shown below:

Problem (A)

$$\min_{x_1,x_2} \phi = 3x_1 + x_2$$

Subject to

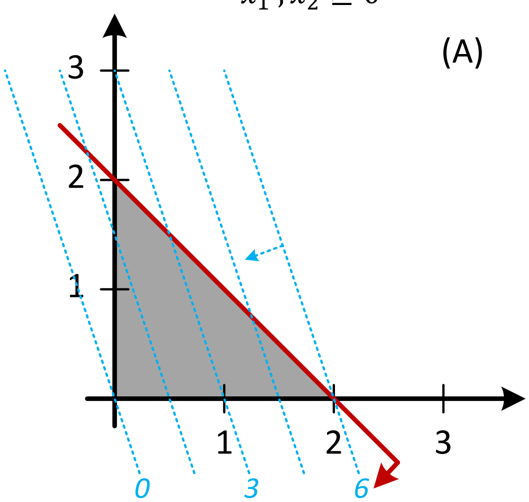
$$x_1 + x_2 \leq 2$$
$$x_1, x_2 \geq 0$$

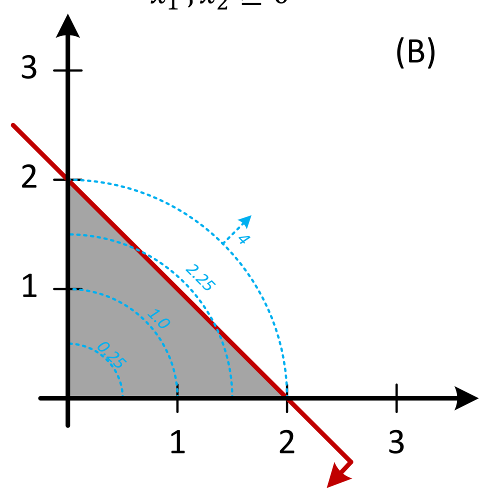
Problem (B)

$$\max_{x_1,x_2} \phi = x_1^2 + x_2^2$$

Subject to

$$x_1 + x_2 \leq 2$$
$$x_1, x_2 \geq 0$$





8.2.9. Optimization Outcomes

The Optimum

An optimum solution $\boldsymbol{x}^\star$ to an optimization problem is a *feasible* choice of the decision variables with an objective function value ϕ *at least* as low (high) as any other solution satisfying the constraints:

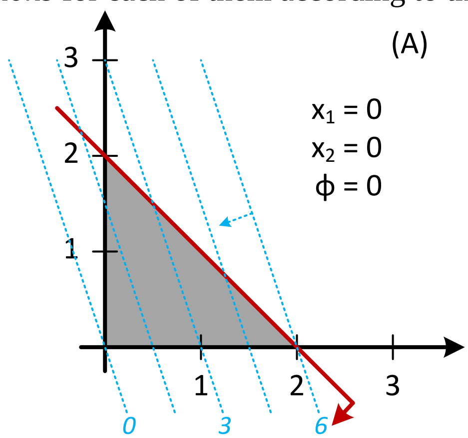
$$\phi(\boldsymbol{x}^\star) \leq (\geq)\, \phi(\boldsymbol{x}) \quad \forall\, \boldsymbol{x} \in \mathcal{S}$$

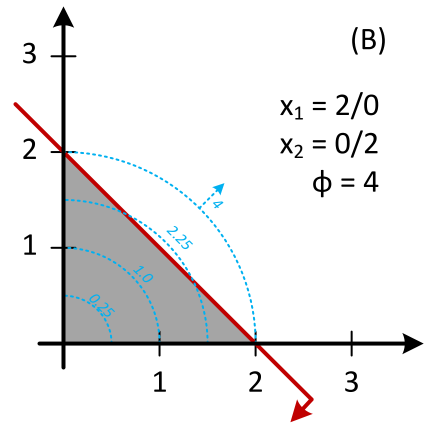
We will get into more detailed definitions of optimality later.

As far as nomenclature and graphical solutions are concerned, please consider the following **remarks**:

- Optimal solutions are shown graphically to be the point(s) lying on the best objective function contour that intersects with at least one boundary of the feasible region.
- The *optimal value* $\phi^\star$ is defined to be the value of the objective at the optimum(s): $\phi^\star \triangleq \phi(\boldsymbol{x}^\star)$.
- An optimization model can have only **one** true optimal value. It may have:
    - A **unique** optimal solution.
    - Several **alternative** solutions $\boldsymbol{x}^\star$ yielding the *same* optimal $\phi^\star$.
    - **No** optimal solutions (either the problem is unbounded or infeasible).

For example, considering the same optimization problems as above, we can identify the *optimal solutions* for each of them according to the plots below:





However, we run into situations of **degeneracy** and **unboundedness** when we slightly modify the problem as follows:

Problem (A)

$\max_{x_1,x_2} \phi = 3x_1 + 3x_2$

Subject to

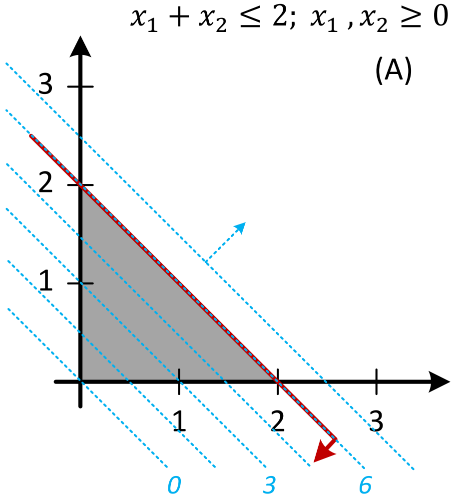
$x_1 + x_2 \leq 2;\ x_1\,, x_2 \geq 0$

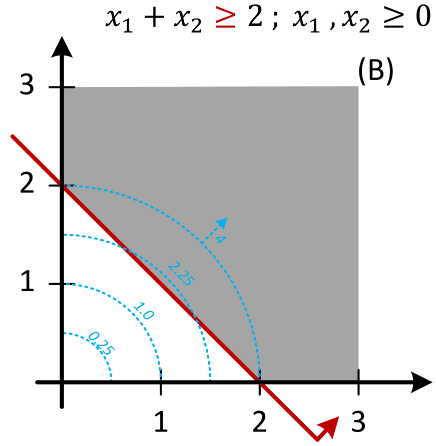
Problem (B)

$\max_{x_1,x_2} \phi = x_1^2 + x_2^2$

Subject to

$x_1 + x_2 \geq 2\,;\ x_1\,, x_2 \geq 0$





Active Constraints

A constraint $g(\boldsymbol{x}) \leq 0$ is said to be:

- **Active** (or **binding**) at some point $\boldsymbol{x}^\star$ if $g(\boldsymbol{x}^\star) = 0$.
- **Inactive** at some point $\boldsymbol{x}^\star$ if $g(\boldsymbol{x}^\star) < 0$.

And finally, consider the following **remarks** regarding active constraints:

- The set of constraints that are active at the optimal solution are known as the **active set**.
- Equality constraints are **ALWAYS** active at any feasible optimal point.
- No constraints (inequality or equality) may be violated at any optimal point.

8.2.10. Graphing Example: Crude Distillation

Let us revisit the crude distillation question. Recall the problem formulation:

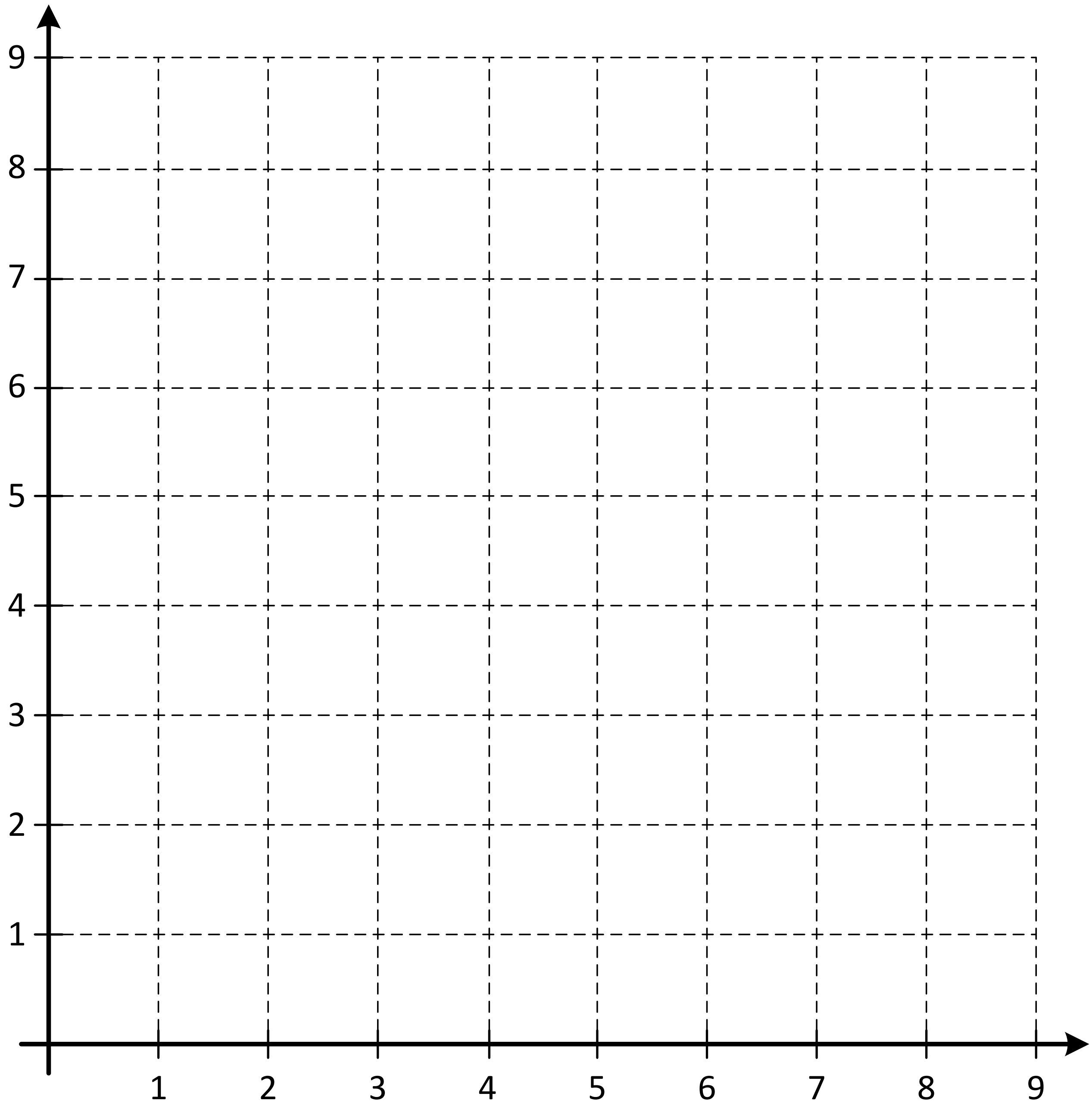
$$\min_{x_1, x_2} \phi = 50x_1 + 37.5x_2$$

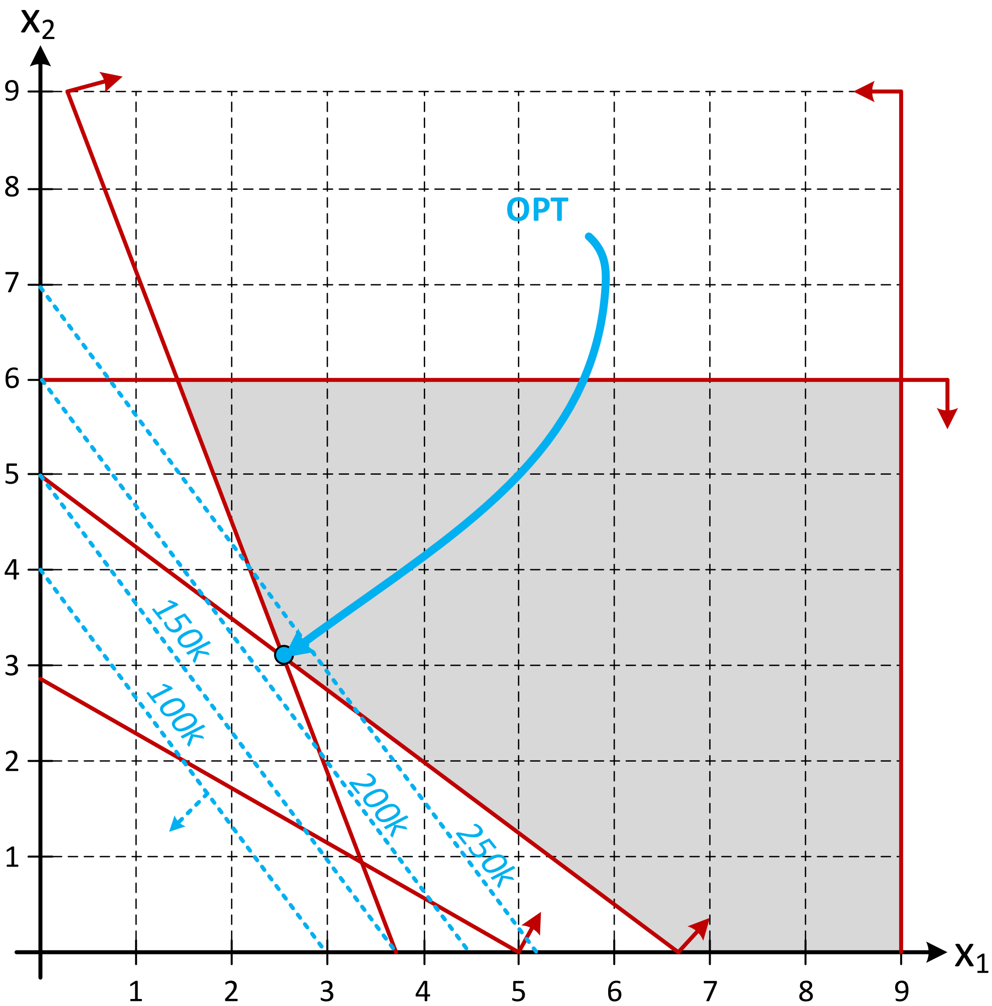
Subject to

$$\begin{aligned}
0.3x_1 + 0.4x_2 &\geq 2{,}000 \\
0.4x_1 + 0.15x_2 &\geq 1{,}500 \\
0.2x_1 + 0.35x_2 &\geq 1{,}000 \\
x_1 &\leq 9{,}000 \\
x_2 &\leq 6{,}000 \\
x_i &\geq 0
\end{aligned}$$

On the graph paper below, plot the model constraints, objective contour, and identify the optimum. Solution will be taken up in class.

Graphical Optimization of Crude Distillation Example





8.3. Conclusions

We now have a good handle on the formulation of optimization problems. Formulation and graphical solutions are **imperative** to enhance one's understanding of the types of problems we may encounter, and how to turn real-world opportunities into formal mathematical programs that we can handle.