# 4. Optimization Definition and Formulation

## 4.1. Introduction

In Part 1 of this book, we discussed the basics of surrogate modeling using polynomial response surfaces. In most engineering applications, surrogate modeling is not a goal but a tool. The purpose of surrogate modeling is to construct an approximate model such that the cost of experiments or simulations can be reduced in subsequent analysis. Therefore, the effectiveness of a surrogate model is increased when an application requires numerous experiments or simulations with different values of input variables. Common applications include design optimization and uncertainty quantification, where hundreds or thousands of simulations are required. This book focuses on design optimization, where input variables represent design variables, and the quantity of interest (QoI) is either the objective or constraint function. Since an approximate model is used, it is referred to as surrogate-based analysis and optimization (SBAO) in this text. In addition to saving computational time, surrogates also allow for the optimization of applications with non-smooth or noisy responses and can provide insight into the nature of the design space [38].

In order to understand the basic procedure and concept of SBAO, it would be necessary to discuss design optimization first. Part 2 of this book will discuss the fundamentals of design optimization. The contents of this part are by far brief and incomplete. We will define basic terminologies that are used in design optimization and basic algorithms to solve optimization problems. For a comprehensive understanding of design optimization, users are referred to the books of Arora [39] and Haftka and Gürdal [40].

As a first step toward design optimization, this chapter will present the definition of design optimization, optimization formulation, and optimality criteria. First, we will define the design optimization definition in Section 4.2, where various terminologies in optimization are defined. The definition of an optimization problem boils down to defining design parameters, objective functions, and constraint functions. When the number of design variables is less than two, graphical optimization is also presented. In Section 4.3, the standard form of an optimization problem is introduced, which makes it possible for engineers to focus on solving optimization problems in a unified fashion. The concept of convexity is briefly introduced as well, which can guarantee the global optimum design. In Section 4.4, an important topic of optimality criteria is presented, which leads engineers to find an optimum design. In practice, optimality criteria are used to determine if a given design is an optimum design or not.

## 4.2. Design optimization definition

Design is a procedure to improve or enhance the performance of a system by changing its parameters. In the previous chapters, the performance of a system is referred to as a quantify of interest (QoI). A QoI can be quite general in engineering fields and can include: the weight, stiffness, and compliance of a structure; the fatigue life of a mechanical component; the noise in the passenger compartment; the vibration level; the output power of a generator; the safety of a vehicle in a crash, etc. However, aesthetic measures such as whether a design is attractive to customers are not considered. All QoIs are presumed to be measurable quantities. System parameters are variables that a design engineer can change during the design process. For example, the thickness of a vehicle body panel can be changed to improve vehicle performance. The cross-section of a beam can be changed in designing bridge structures. System parameters that can be changed during the design process are called design variables.

*Design optimization process*

The engineering design of a system in the simulation-based design process consists of design problem formulation, mathematical modeling, parameterization, simulation, and optimization. Figure 4-1 is a flow chart of the design optimization process in which computational simulation and mathematical programming (optimization algorithm) play essential roles. The success of the system-level, simulation-based design process strongly depends on consistent design parameterization, an accurate simulation, and an efficient mathematical programming algorithm.

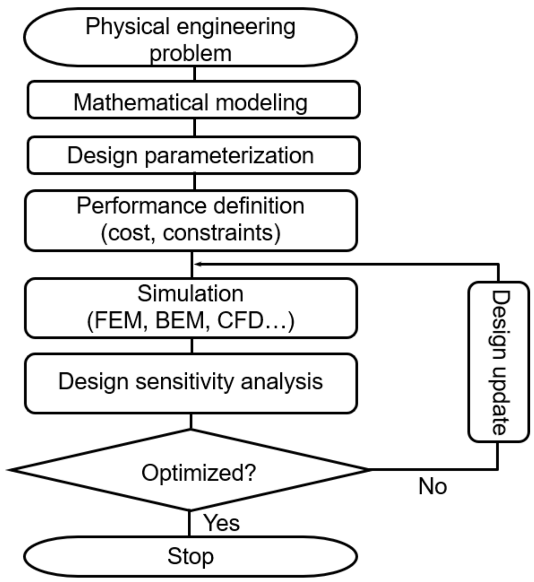


Figure 4-1: Flowchart of the design optimization process.

A design engineer simplifies a physical engineering problem into a mathematical model that can represent the physical problem up to the desired level of accuracy. A mathematical model has parameters that are related to the parameters of the physical problem. Among them, the design engineer identifies those design variables to be used during the design process. Design parameterization, which allows the design engineer to define the properties of each design component of the system being designed, is one of the most important steps in the design process. The principal role of design parameterization is to define the system parameters that characterize the system model and to collect a subset of the parameters as design variables. Design parameterization forces engineering teams in design, analysis, and manufacturing to interact at an early design stage, and supports a unified design variable set to be used as the common ground to carry out all simulations, design, and manufacturing processes. Only proper design parameterization will yield a good optimum design since the optimization algorithm will search within a design space that is defined for the design problem. The design space is defined by the type, number, and range of design variables.

Simulation can be carried out using experiments on an actual or reduced scale, which is a straightforward and still prevalent method for industrial applications. However, the expense and the inefficiency involved in fabricating prototypes make this approach difficult to apply. An analytical model may resolve these difficulties since it approximates the physical problem as a mathematical model and solves it in a simplified form. However, the analytical method has limitations even for very simple problems. With the emergence of various computational capabilities, most analytical approaches to mathematical problems have been converted to numerical approaches, which can solve very complicated, real engineering applications. Finite element analysis (FEA), boundary element analysis, and computational fluid dynamics (CFD) are a short list of numerical tools used in engineering analysis. However, the numerical models themselves can be computationally expensive and may include numerical errors. The main purpose of surrogate modeling is to replace the numerical simulation with a surrogate model such that the computational cost can be reduced significantly.

The selection of a design space and an analysis method must be carefully determined since the analysis, both in terms of accuracy and efficiency, must be able to handle all possible designs in the chosen design space. That is, the larger the design space, the more sophisticated the analysis capability must be. For example, if larger shape design changes are expected during design optimization, mesh distortion in FEA could be a serious problem and a finite element model that can handle large shape design changes must be used.

A performance measure in a simulation-based design is the result of numerical simulations. Based on the evaluation of simulation results, such engineering concerns as high stress, clearance, natural frequency, output torque, or mass can be identified as performance measures for design improvement. Typical examples of performance measures are mass, volume, displacement, stress, compliance, buckling, natural frequency, noise, fatigue life, and crashworthiness. It is expected that the users should define all relevant performances that are of concern during the design process.

Cost and constraints can be defined by combining certain performance measures with appropriate constraint bounds for interactive design optimization. The cost function, sometimes called the objective function, is minimized (or maximized) during optimization. The selection of a proper cost function is an important decision in the design process. A valid cost function has to be influenced by the design variables of the problem; otherwise, it is not possible to reduce the cost by changing the design. In many situations, an obvious cost function can be identified. In other situations, the cost function is a combination of different performance measures. This is called multi-objective cost functions. The contribution of different cost functions must be either weighted or traded-off.

Constraint functions are the criteria that the system has to satisfy for each feasible design. Among all design ranges, those that satisfy the constraint functions are candidates for the optimum design. For example, a design engineer may want to design a bridge whose weight is minimized and whose maximum stress is less than the yield strength. In this case, the cost function, or weight, is the most important criterion to be minimized. However, as long as stress, or constraint, is less than the yield strength, the stress level is not important.

Once the design variables, cost, and constraint functions are defined, an optimization engine starts changing the design variables to find the best cost function that satisfies all constraint functions. This is an iterative process, which requires numerous evaluations of functions. Surrogate models can play a critical role in this stage to approximate the expensive function evaluations with cheap surrogate models. In general, optimization algorithms are categorized into gradient-based and gradient-free algorithms. Most gradient-based optimization algorithms are based on the mathematical programming method, which requires the function values and gradient (i.e., sensitivity) information at given design variables. For a given design variable that defines the numerical model, simulation provides the values of the cost and constraint functions for the algorithm. The sensitivities of the cost and constraint functions must also be supplied to the optimization algorithm. Then, the optimization algorithms calculate the best possible design for the problem. Chapter 5 will introduce several numerical optimization algorithms. Each algorithm has its own advantages and disadvantages. The performance of an optimization algorithm critically depends on the characteristics of the design problem and the types of cost and constraint functions. Since most gradient-based algorithms try to improve the design by searching nearby designs starting from the current design using gradient information, the search is limited to finding local minima.

In addition, the mathematical programming algorithms assume that both the cost and constraint functions are smooth and continuous functions of design variables.

The main difference between gradient-based and gradient-free algorithms is the requirement of gradient information, which tends to be expensive and sometimes difficult to calculate. The gradient-free algorithms explore the design space to find a better design. Therefore, they have a better chance to find the global minimum. However, there is no guarantee that gradient-free algorithms can find the global minimum. The main bottleneck of gradient-free algorithms is that the number of function evaluations is often too many, which is the main advantage of surrogate modeling. Therefore, gradient-free algorithms are popular in conjunction with surrogate models. In Chapter 6, several popular gradient-free optimization algorithms will be introduced, such as the genetic algorithm, particle swarm optimization algorithm, and direct search algorithm.

*Design variables and feasible domain*

Design variables are those system parameters that design engineers want to change during the optimization process. Theoretically, any system parameter can be a design variable, but the process and performance of optimization strongly depend on the types of design variables. The optimization engine generates a set of design variables that require performance values from simulation and sensitivity information to find an optimum design. Thus, the numerical model has to be updated for a different set of design variables supplied by the optimization engine. If the cost function reaches a minimum with all constraint requirements satisfied, then an optimum design is obtained.

Common design variables include material properties, boundary and loading conditions, the thickness of a plate, cross-sectional dimensions of a beam, and the shape of a domain. Many design variables are related to the geometry of a system, but there are also mathematical quantities, such as the stiffness of a spring, and the damping coefficient of a dashpot, which can be served as design variables. From the perspective of mathematical programming, the most important characteristic of design variables is continuous or discrete. A continuous design variable can take any value between the lower- and upper-bounds in real space. However, discrete variables can only take a specific set of candidates. For example, if the number of students is a design variable, then it is inherently a discrete variable. Another important characteristic of design variables is independence; That is, design engineers can change all design variables independently. A common example is shown in Figure 4-2, where the cross-sectional dimensions of the tube are defined as design variables. In this case, three variables, $r_o, r_i$, and $t$, are not independent because there exists a relationship $t = r_o - r_i$. Therefore, design engineers cannot change all three variables independently.

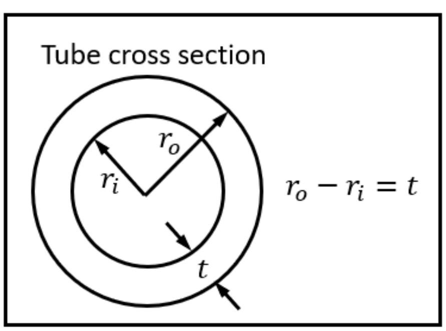


Figure 4-2: Independence of design variables.

The purpose of an optimization problem is to find the best design among many possible candidates. For this reason, design engineers have to specify the best possible design as well as the best possible candidates. Although the design space is given, not all designs in the design space can be a candidate because some of them may not satisfy constraints. The subset of design space that satisfies all constraints is called a feasible set. Mathematically, the feasible set $S$ is defined as

$$S = \{\mathbf{x} \mid \mathbf{x} \text{ satisfies all constraints}\} \tag{4.1}$$

A possible candidate must exist within a feasible design region to satisfy problem constraints. Every design in the feasible region is an acceptable design, even if it is not the best one. The best design is usually the one that minimizes (or maximizes) the cost function within the feasible set. Thus, the goal of the design optimization problem is to find a design that minimizes the cost function among all feasible designs.

**Example 4-1**

In Chapter 2, we discussed the least-squares method, where the error between the samples and surrogate prediction is minimized. This is indeed an optimization problem. Consider fitting the stress-strain relationship $\sigma = E\epsilon$ using the following three measured samples:

| | | | |
|---|---|---|---|
| Strain ($\mu\epsilon$) | 1 | 2 | 4 |
| Stress ($ksi$) | 1 | 2 | 3 |

Find Young's modulus $E$ which minimizes the difference between the samples and the model using (a) the maximum difference and (b) the root-mean-squares (RMS) difference.

**Solution**:

The goal is to find Young's modulus $E$ which minimizes the differences between the samples and the model. In this case, the design variable is Young's modulus $E$, and the objective function is the goodness of fit. For a given Young's modulus $E$, it is possible to define three errors between the samples and the curve. It is clear when we say the best fit, we want all three errors to be small. However, if we want a single measure of goodness, we need to obtain a single measure of the smallness of the three errors. As we discussed in Chapter 2, different measures can be used for the goodness of fit. Therefore, the following two different optimization problems can be formulated:

Maximum difference

$$d_{max}(E) = \max_{i=1,2,3} |\sigma_i - E\epsilon_i|$$

RMS

$$d_{RMS}(E) = \sqrt{\frac{1}{3}\sum_{i=1}^{3}(\sigma_i - E\epsilon_i)^2}$$

(a) In the case of maximum difference, the minimum $d_{max}(E)$ occurs when the maximum positive difference is in equal magnitude with the maximum negative difference. For the given samples, this occurs between the second and the third samples (the difference in the first sample is always less than that of the second sample). Therefore, the minimum $d_{max}(E)$ occurs when $2 - 2E = -(3 - 4E)$, which yields $E_{max} = 5/6\ ksi/\mu\epsilon$.

(b) In the case of RMS difference, the square of $d_{RMS}$ can be written as

$$d_{RMS}^2(E) = \frac{1}{3}[(1-E)^2 + (2-2E)^2 + (3-4E)^2] = \frac{1}{3}(14 - 34E + 21E^2)$$

The $d^2_{RMS}(E)$ has its minimum when its derivative with respect to $E$ becomes zero; that is, $E_{RMS} = 17/21\ ksi/\mu\epsilon$.

It is noted that the two formulations yield different optimum designs. Therefore, it is important to define the cost function carefully as the optimum design depends on how the cost function is defined. In practice, the RMS difference is popular because the cost function is a smooth (nonlinear) function of design variables such that the maximum/minimum can be found using gradient information. Figure 4-3 shows the optimization results using the two different cost functions. $E_{RMS}$ is slightly lower than $E_{max}$ because the first data does not have any role in the maximum difference cost function. Also, the figure shows that $d_{max}$ is not continuous at the optimum design, while $d_{RMS}$ is continuous. The following Matlab code is used to generate the plot in Figure 4-3:

```
eps=[1 2 4]; sig=[1 2 3];
e=linspace(0.5,1,101);
sigmodel=e'*eps;
sigr=ones(101,1)*sig;
diff=abs(sigr-sigmodel);  maxdiff=max(diff');
sumsquares=diag(diff*diff');  rms=sqrt(sumsquares/3);
plot(e,maxdiff); xlabel('E'); ylabel('cost function')
hold on;  plot(e,rms,'r-'); legend('max error','RMS
error','Location','North')
```

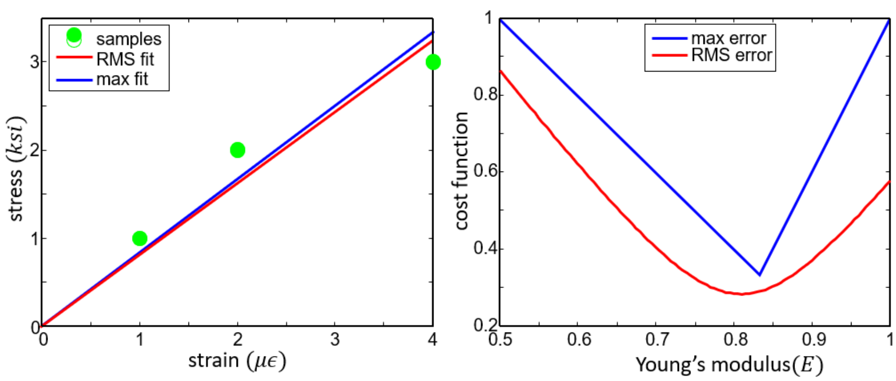


Figure 4-3: Stress-strain curve and the variation of the cost function.

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**Example 4-2**

The weight and value of the five items are shown in the table. We want to put items in the knapsack to maximize the total value while the total weight is less than 20 lbs. Define the optimization problem; i.e., define design variables and cost function.

| Item | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| Weight (lb) | 4 | 6 | 7 | 10 | 3 |
| Value ($) | 12 | 12 | 12 | 27 | 5 |

**Solution**:

In this case, design variables would be if an item is chosen or not. Therefore, the design variables are not continuous, but discrete. Indeed, design variables are binary. If $i$th item is chosen, the design variable $x_i = 1$, otherwise, $x_i = 0$. The cost function is the total value of the chosen items. However, since the total weight must be less than 20 lbs, the cost is reduced by \$10 if the total weight is over 20 lbs. This obviously may not prevent the total weight of over 20 lbs, but we will use this approach for the moment. Therefore, the objective function can be written as

$$\underset{x_i \in (0,1)}{\text{maximize}} \quad \text{value} = 12(x_1 + x_2 + x_3) + 27x_4 + 5x_5$$
$$-10 \times \text{sgn}(4x_1 + 6x_2 + 7x_3 + 10x_4 + 3x_5 - 20)$$

where sgn() is a signum function, whose value is one if the argument is greater than zero, otherwise zero.

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The previous two examples are referred to as unconstrained optimization because the optimization problem has only an objective function, but no constraints. Of course, there is a constraint for a design variable, such as binary design or lower- and upper-bounds of design variables. However, these types of constraints can be handled directly when the design variable is changed. Therefore, they are referred to as side constraints.

The condition of the total weight being less than 20 lbs in **Example 4-2** can be written in the form of a constraint. In this case, the constrained optimization problem can be written as

$$\underset{x_i \in (0,1)}{\text{maximize}} \quad \text{value} = 12(x_1 + x_2 + x_3) + 27x_4 + 5x_5$$
$$\text{subject to} \;\; 4x_1 + 6x_2 + 7x_3 + 10x_4 + 3x_5 \le 20$$

In practice, there are many different ways of formulating an optimization problem. For example, the optimization problem in **Example 4-1** yields a smooth objective function in the case of RMS difference. However, in the case of maximum difference, the objective function becomes non-smooth. To avoid a non-smooth objective function, we can add a bound design variable $\alpha$, as well as error bound constraints, such that the following constrained optimization problem is equivalent to the one that was defined in **Example 4-1**:

$$\underset{\alpha, E}{\text{minimize}} \quad \alpha$$
$$\text{subject to} \; -\alpha \le \sigma_i - E\epsilon_i \le \alpha, \quad i = 1,2,3$$

The optimization problem has three constraints. It is noted that the objective function is equal to one design variable, $\alpha$, and the other variable $E$ appears only in the constraints. It is also noted that both the objective and constraint functions are smooth and linear. Since we know the sign of the differences, we can rewrite the optimization problem as

$$\underset{\alpha, E}{\text{minimize}} \quad \alpha \tag{4.2}$$
$$\text{subject to} \; \sigma_1 - E\epsilon_1 \le \alpha, \sigma_2 - E\epsilon_2 \le \alpha, \sigma_3 - E\epsilon_3 \ge -\alpha$$

Therefore, by introducing an additional variable, $\alpha$, it is possible to make the objective and constraint functions smooth. We will discuss how to define an optimization problem in Section 4.3 in detail.

*Graphical optimization*

In general optimization problems, it is difficult to see the relationship between objective and constraint functions with respect to design variables because the number of design variables is usually large. Therefore, visualizing objective and constraint functions in high dimensions is a challenging task. However, when the number of design variables is one or two, it is possible to plot the objective and constraint functions and find the optimum design graphically. Since graphical optimization plots all functions in the entire design space, it is expensive but helps to visualize the design space and to understand the nature of the design problem. The procedures of graphical optimization are as follows:

- Draw the design space (lower- and upper-bounds of design variables)
- Plot constraints on the graph and find the feasible set
- Plot contour lines of the objective function
- Find the optimum point (the objective function has the lowest value within the feasible set)

The following example illustrates the graphical optimization for finding Young's modulus in **Example 4-1** using the constrained optimization problem in Eq. (4.2).

**Example 4-3**
Find the optimum Young's modulus of **Example 4-1** using the constrained optimization problem in Eq. (4.2).

**Solution**:
The optimization problem in Eq. (4.2) is linear in the sense that both the objective function and constraint functions are linear functions of design variables. The three inequality constraints are shown in Figure 4-4 where colored lines are constraint boundaries with hatching marking the region where the constraint is violated. This is a standard way of marking an inequality constraint. The feasible set $S$ is defined as the area that satisfies all constraints. Since the objective function is equal to $\alpha$, there is no need for objective function contours. Within the feasible set, the optimum design that minimize $\alpha$ is the lowest point in the vertical axis, which is Point A in the figure. At optimum design, $E = 5/6$ and the maximum error $d_{max} = 1/3$.

It is seen that there are two active constraints at the optimum design at Point A; they are second (red) and third (green) constraints. It is easy to check that the error at the first constraint is half of that of the second constraint for any value of $E$, so that constraint is not binding. The optimum is found therefore at the intersection, where the differences between the model and the second and third constraints have the same magnitude and opposite signs.

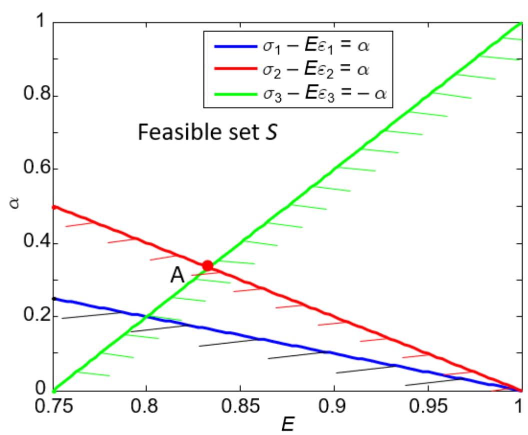


Figure 4-4: Graphical optimization of finding Young's modulus.

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Graphical optimization can provide additional benefits in understanding the optimization problem at hand. When the feasible domain is not well-defined, the optimization problem can have a problem. These problems are often difficult to identify in a high-dimensional design space. However, using graphical optimization, the design space along with all constraints can be visualized, from which possible problems in the feasible domain can be identified first. The possible problems that are related to the feasible domain are (a) problems with unbounded feasible regions, (b) problems with multiple optima, (c) problems with empty feasible regions, and (d) problems with no active constraints. Figure 4-5 shows some examples of problems related to the feasible regions. The blue lines are the contour of the objective function whose values decrease in the direction of $\Delta f < 0$. The red lines are the constraint bounds where the design becomes infeasible on the hatched side. In Figure 4-5(a), the objective function is reduced as the design moves away from the constraint bounds. Therefore, in this problem, the optimum solution is unbounded, and the constraints do not play any role in the optimization problem. In Figure 4-5(b), two constraints conflict with each other, and there is no feasible domain at all. In this case, there is no optimal solution exists. The last difficulty in Figure 4-5(c) is when the contour line of the objective function is parallel to the constraint bound. In this case, all designs along the line PQ can be optimum designs as the objective function has the same value along the line.

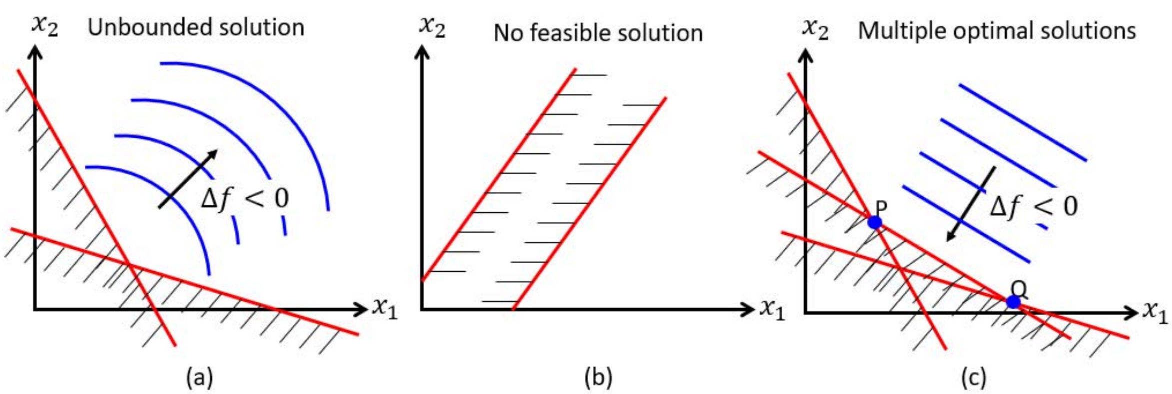


Figure 4-5: Examples of problems with feasible domains.

## 4.3. Optimization problem formulation

Optimization exists in almost all engineering applications. Therefore, instead of developing optimization procedures for different applications, it makes sense to develop a unified optimization procedure that can be used for any application. Such unification can be possible by defining the standard form of optimization problem formulation. We first present the three-step optimization problem definition, which defines the three ingredients of optimization problems. Next, the standard form of an optimization problem is presented. As long as an optimization problem can be written in the standard form, the subsequent optimization procedures can be applied independently of applications. Lastly, the convex optimization problem is presented, which is an important property of an optimization problem.

*Three-step problem definition*

Most engineering optimization problem formulation can be achieved in three steps: design parameterization, defining an objective function, and defining constraint functions. Design parameterization is to define/select design variables from system parameters. Although any parameter can be selected as a design variable, it is important to identify design variables clearly. In addition, as mentioned in the previous section, it is important that all design variables can maintain independence. In this text, the vector of design variables is defined as $\mathbf{x} = \{x_1, x_2, \cdots, x_n\}^T$, where $n$ is the dimension of design variables. In general, design variables can be discrete or continuous. However, in the context of surrogate modeling, since a surrogate model assumes that input variables are continuous and the QoI is a smooth function of input variables, design variables are considered continuous as well. In order to define the design space, it would be necessary to specify the lower- and upper-bounds of each design variable. These bounds are specified by side constraints, $\mathbf{x}_L \le \mathbf{x} \le \mathbf{x}_U$, where $\mathbf{x}_L$ and $\mathbf{x}_U$ are, respectively, the lower- and upper-bounds of design variables.

An objective function must be a function of design variables. In the context of surrogate modeling, the objective function is a continuous and smooth function of design variables. In general, the objective function can be minimized or maximized. However, in the standard form of optimization, it is assumed that the objective function is minimized during the optimization process. When an objective function is supposed to be maximized, the negative objective function is minimized instead. That is,

$$\underset{\mathbf{x}}{\text{maximize}}\, F(\mathbf{x}) \;\; \rightarrow \;\; \underset{\mathbf{x}}{\text{minimize}}\, f(\mathbf{x}) = -F(\mathbf{x})$$

Constraint functions can be given in the form of equality or inequality constraints. The functional requirements of constraint functions are identical to that of the objective function: dependence on design, smoothness, and continuity. The standard form of inequality constraint is less than or equal to zero. That is, $g(\mathbf{x}) \le 0$. However, many engineering applications have constraints in the form that the constraint function is less than (or larger than) a threshold. In such a case, the constraint can be converted into

$$\begin{aligned} g(x) \le g_{max} \;\; &\rightarrow \;\; g(x) - g_{max} \le 0 \\ g(x) \ge g_{min} \;\; &\rightarrow \;\; g_{min} - g(x) \le 0 \end{aligned}$$

The standard form of equality constraint is $h(\mathbf{x}) = 0$. If the right-hand side is not zero, a similar conversion as in the inequality constraint can be done. Although there is no limit to the number of inequality constraints, the number of equality constraints must be less than the number of design variables.

*Standard form*

From the viewpoint of algorithm development, it would be convenient if all optimization problems are written in a single form. Then, the developers do not need to consider solving different optimization problems. To facilitate the description of algorithms for solving optimization problems, there is a fairly standard notation for writing them. The letter $f$ is typically used for objective functions, $g$ for inequality constraints, and $h$ for equality constraints. Lower- and upper-bounds on design variables are often called side constraints and are written separately in different forms. The standard form of an optimization problem in this text is defined as

$$\begin{aligned} &\text{minimize} \;\; f(\mathbf{x}) \\ &\text{subject to}\; g_i(\mathbf{x}) \le 0, \qquad i = 1, \cdots, K \\ &\qquad\qquad h_j(\mathbf{x}) = 0, \qquad j = 1, \cdots, M \\ &\qquad x_l^L \le x_l \le x_l^U, \qquad l = 1, \cdots, n \end{aligned} \tag{4.3}$$

where $\mathbf{x} = \{x_1, x_2, \cdots, x_n\}^T$ is the vector of design variables, $f(\mathbf{x})$ is the objective function, $g_1(\mathbf{x}), \cdots, g_K(\mathbf{x})$ are inequality constraints, $h_1(\mathbf{x}), \cdots, h_M(\mathbf{x})$ are equality constraints, and $\mathbf{x}^L$ and $\mathbf{x}^U$ are lower- and upper-bounds of design variables, respectively. Of course, not all optimization problems can be written in standard form. For a more general form of optimization problems, the readers are referred to the paper published by Svanberg [41]. Once the inequality and equality constraints are all defined, the feasible set in Eq. (4.1) can be written as

$$S = \left\{\mathbf{x} \middle|\, g_i(\mathbf{x}) \le 0, i = 1, \cdots, K; h_j(\mathbf{x}) = 0, j = 1, \cdots, M\right\} \tag{4.4}$$

Therefore, the optimization problem is to find the optimum design variable $\mathbf{x}^* \in S$ that minimizes the objective function $f(\mathbf{x}^*)$.

When an inequality constraint is strictly less than zero, i.e., $g_i(\mathbf{x}) < 0$, the constraint is inactive. When the constraint is on the bound, $g_i(\mathbf{x}) = 0$, it is active. Lastly, the constraint is violated when $g_i(\mathbf{x}) > 0$. On the other hand, an equality constraint can be either active, $h_j(\mathbf{x}) = 0$, or violated, $h_j(\mathbf{x}) \neq 0$. In general, when all constraints are linearly independent, the total number of active constraints should be less than or equal to the number of design variables. This can be understood from the basic law of linear algebra, where the number of independents equation cannot be more than the number of unknown variables.

Optimization problems can be categorized depending on the functional form of the objective and constraint functions. First, when both the objective function and all constraint functions are linear functions of design variables, it is called a linear programming (LP) problem. In such a case, many specialized numerical algorithms are available. A quadratic programming (QP) problem occurs when the objective function is a quadratic function of design variables, while all constraints are linear. As we will discuss in the next subsection, the global optimum design can be found when the optimization problem is LP or QP. When both objective function and constraint functions are a nonlinear function of design variables, it is called nonlinear programming (NLP) problem, which is the most general but at the same time most challenging to find the optimum design.

*Normalization*

Even if an optimization problem is well defined in the standard form, it may cause some numerical difficulties to solve. This is because engineering optimization may cover a broad range of quantities of interest. Different objectives and constraints may have different orders of magnitude. For example, the allowable strength of steel is about 500 MPa, which is $5 \times 10^8$ Pa. On the other hand, the allowable displacement can be in the order of $10^{-3}$m. When the objective and constraint functions have a huge difference in magnitude, the standard form has no problem from the mathematical viewpoint, but it is numerically difficult to handle such a huge difference in the orders of magnitude. Therefore, it makes sense to normalize the objective and constraints such that their magnitude is approximately in the order of one. For example, stress constraint is often given in the form of $\sigma_{max} \leq \sigma_{allowable}$. Then it is possible to normalize the constraint using $\sigma_{allowable}$ and make it in the standard form as

$$\frac{\sigma_{max}}{\sigma_{allowable}} - 1 \leq 0 \tag{4.5}$$

Since all constraints have their limits, they can be normalized using their limits. In the case of the objective function, it can be normalized using its initial value or using the target value.

**Example 4-4**
Write the standard form of the optimization problem in **Example 4-3**.

**Solution**:
The optimization problem formulation given in Eq. (4.2) is not the standard form. Without normalizing the objective and constraints, the standard form of the optimization problem can be written as

$$0.5 \leq E \leq 1$$

Note that the side constraint is added to limit Young's modulus. Note that the normalization of this optimization problem can be tricky. Since the limit of inequality constraints, $\alpha$, is not fixed but a design variable itself. Therefore, in this case, it would be better not to normalize the optimization problem.

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**Example 4-5**

A tubular column is under the compressive load $P$ as shown in the figure. The height of the tube is fixed, and the mid radius $R$ and thickness $t$ are design variables. The goal is to minimize the weight of the tube, which is equivalent to the cross-sectional area of the tube. The following three failure modes are considered constraints. (a) Stress failure: the axial compressive stress should be less than the allowable strength $\sigma_a$. (b) Global buckling: the tube should not buckle for the given applied load $P$. (c) Local buckling: the tube should not wrinkle into a diamond pattern as shown in the figure. The design variables have lower- and upper-bounds. Write the standard form of the optimization problem.

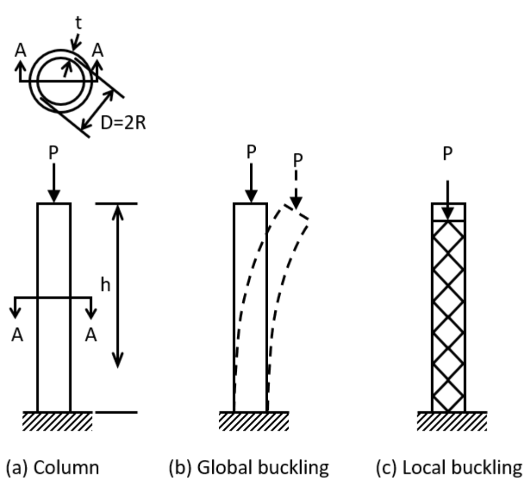


Figure 4-6: A tube under compressive load.

**Solution**:

Assuming that the radius is much larger than the thickness, $R \gg t$, the cross-sectional area and the moment of inertial can be approximated as $A = 2\pi Rt$ and $I = \pi R^3 t$. Then, the objective function can be defined using the density of the material and the volume of the tube as

$$mass = \rho(hA) = 2\pi\rho hRt$$

The equations for the three failure modes are given as

$$\text{Stress constraint: } \sigma = \frac{P}{2\pi Rt} \leq \sigma_a$$

$$\text{Buckling load: } P_{cr} = \frac{\pi^3 E R^3 t}{4h^2} \geq P$$

$$\text{Local buckling: } \sigma_s = \frac{2Et}{2R\sqrt{3(1-\nu^2)}} \leq \sigma_a$$

$$\text{Side constraints: } R_{min} \leq R \leq R_{max}, \qquad t_{min} \leq t \leq t_{max}$$

Each failure mode provides for different importance of the diameter and the thickness. The stress depends only on the area, which is also the objective function, and the area depends only on the product of the thickness and the diameter. This means that with a stress constraint only, any combination of the diameter and thickness that is at the stress limit $\sigma_a$ will have the same weight.

The global buckling load depends on the Moment of inertia $I$ that depends on $D$ more strongly than on $t$. Therefore, it will drive the design toward a thin tube. Local buckling pushes in the other direction in that it benefits from large $t$ and small $D$. This indicates that if buckling is critical (happens if the column is slender enough, i.e. $h$ is large), both failure modes will happen simultaneously.

The standard formulation requires us to write the failure constraints so that all are of the form $g(D,t) \le 0$. Therefore, the standard form of the optimization problem can be written as

$$\begin{aligned} \underset{R,t}{\text{minimize}} \quad & 2\pi\rho hRt \\ \text{subject to} \quad & g_1(R,t) = \frac{\sigma}{\sigma_a} - 1 \le 0 \\ & g_2(R,t) = 1 - \frac{P}{P_{cr}} \le 0 \\ & g_3(R,t) = \frac{\sigma_s}{\sigma_a} - 1 \le 0 \\ & R_{min} \le R \le R_{max}, t_{min} \le t \le t_{max} \end{aligned}$$

Also, all constraints are normalized by their limits. This provides a handy measure of constraint satisfaction. For example, if the constraint is equal to $-0.1$, it tells us that we have a 10% margin between the response and the allowable response. If the constraint is equal to 0.05, it means we exceed the allowable by 5%. This normalized and non-dimensional formulation of constraints is also typically better for the numerical performance of optimization algorithms. That is, using an optimization routine, it is likely to lead to faster convergence and increase the chance that we will find the true optimum.

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**Example 4-6**

A beer company wants to design a new can size so that the minimum amount of sheet metal can be used. This is equivalent to minimizing the manufacturing cost. The can is required to hold at least 400 ml of fluid. The diameter of the can should be no more than 8 cm. In addition, it should not be less than 3.5 cm for shipping and handling reasons. The height of the can should be no more than 18 cm and no less than 8 cm. Write the standard form of the optimization problem and solve it using the graphical optimization method.

**Solution**:

As shown in Figure 4-7, the design variables are the diameter $D$ and the height $H$. The amount of sheet metal is the surface area of the can, which is $\pi DH + \pi D^2/2$. The volume of the can is defined in terms of design variables as $\pi D^2 H/4$. Therefore, the standard form of the optimization problem can be written as

$$\begin{aligned} \underset{D,H}{\text{minimize}} \quad & \pi DH + \pi D^2/2 \\ \text{subject to} \quad & 400 - \frac{\pi D^2 H}{4} \le 0 \ \ cm^3 \\ & 3.5 \le D \le 8 \, cm \\ & 8 \le H \le 18 \ \ cm \end{aligned}$$

Note that the inequality constraint is not normalized. Figure 4-7(b) shows the feasible set that satisfies the inequality constraint.

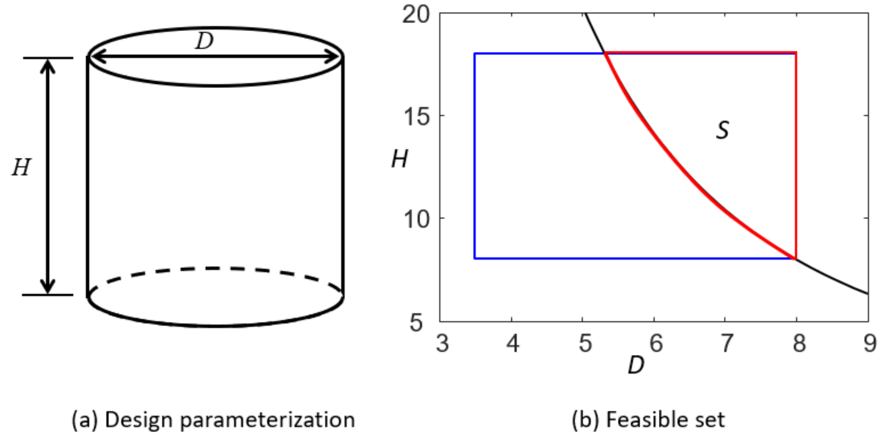


Figure 4-7: Beer can design parametrization and feasible set.

The objective function is a quadratic function of $D$ and a linear function of $H$. As shown in Figure 4-8, the objective function gradually increases as both design variables increase. However, there is no feasible region for $f = 200$. When $f = 300$, the objective contour meets a corner of the feasible set the first time. This point $(D, H) = (8,8)$ is indeed the optimum design. Therefore, the diameter is at its upper-bound, while the height is at its lower-bound.

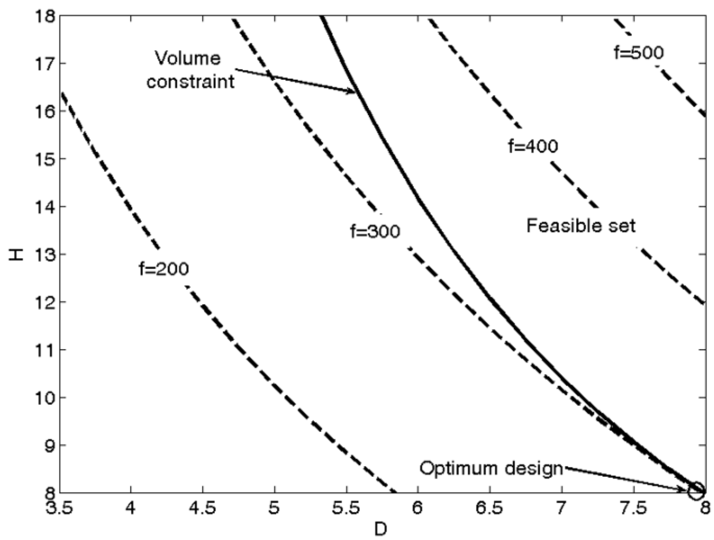


Figure 4-8: Graphical optimization of a beer can design problem.

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*Convex function and convex problem*

The optimization problem formulation defined in the previous subsection is general enough that it can be applied to many engineering applications. However, it does not guarantee that there is a single optimum design especially when the objective and constraints are a nonlinear function of design variables. In fact, an important challenge in numerical optimization is to find the global optimum design. As we will discuss in the next section, most optimization algorithms are designed to find a local optimum, not the global one. However, if a function is convex, it has a single minimum, and the local minimum is the global minimum. Therefore, the concept of a convex function and a convex problem is important as it can provide a nice theoretical foundation to determine the uniqueness of the global optimum design.

A function is convex if a straight line connecting two points on its graph will not dip below the function values in between. That is, the straight line that connects two points on the function is always larger than the function itself. As shown in Figure 4-9(a), for $0 \le \alpha \le 1$, $x = \alpha x^{(2)} + (1-\alpha)x^{(1)}$ is a point between two points $x^{(1)}$ and $x^{(2)}$. Then a function is convex if it satisfies the following condition for all $x$:

$$f(x) \le \alpha f\left(x^{(2)}\right) + (1-\alpha) f\left(x^{(1)}\right) \tag{4.6}$$

The left-hand side is the function value at $x$, while the right-hand side is the straight line that connects $f\left(x^{(1)}\right)$ and $f\left(x^{(2)}\right)$. This can apply to $n$-dimensional function rather than just to a function of a single variable as shown in the figure. The weighted sum of all the quantities, where the sum of the weights is equal to one and all the weights are positive is called a convex combination. Therefore, the equation above says that the value of the function at a convex combination of two points cannot be larger than the convex combination with the same weights of the function values at these two points.

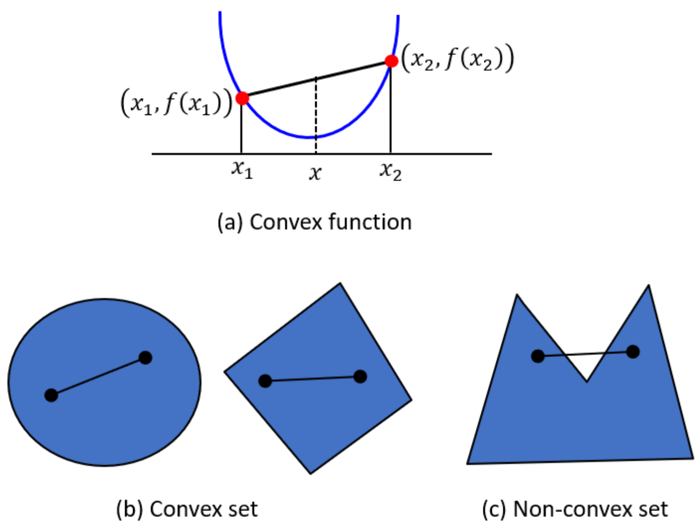


Figure 4-9: Convex function and convex set.

Although the convexity of a function is defined using Eq. (4.6), it is not a convenient form to show convexity because it is impractical to show it for all arbitrary combinations of $x^{(1)}$ and $x^{(2)}$. In practice, convexity is shown using the Hessian information. In multi-dimensional function, let the vector of input variables is defined as $\mathbf{x} = \{x_1, x_2, \cdots, x_n\}^T$. Then, the gradients (first-order derivatives) of function $f(\mathbf{x})$ can be defined as

$$\nabla f(\mathbf{x}) = \left\{\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \cdots, \frac{\partial f}{\partial x_n}\right\}^T \tag{4.7}$$

which is an $n$-dimensional vector. The gradients are the slope of the function in the direction of each variable. The second derivatives of function $f(\mathbf{x})$ are called the Hessian matrix, which is defined as

$$\mathbf{H} \equiv \nabla^2 f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \tag{4.8}$$

The Hessian matrix is symmetric. The Hessian matrix is related to the curvature of the function.

A symmetric matrix $\mathbf{H}$ is positive definite if $\mathbf{x}^T\mathbf{H}\mathbf{x} > 0$ for all $\mathbf{x} \neq 0$. A symmetric matrix is positive semi-definite if $\mathbf{x}^T\mathbf{H}\mathbf{x} \geq 0$ for all $\mathbf{x} \neq 0$. This property is important for the Hessian matrix. If the Hessian matrix $\nabla^2 f$ is positive semi-definite, then the original function $f(\mathbf{x})$ is convex. In addition, if the Hessian matrix is positive definite, then the function $f(\mathbf{x})$ is strictly convex. That is, the function has a single minimum, which is the global minimum.

In order to apply the above concept of convex function to an optimization problem, it is necessary to adopt the concept of a convex set as well because an optimization problem is to minimize the objective function within the feasible set. A feasible set is convex if for all $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ in the feasible set $S$, the convex combination $\mathbf{x} = \alpha\mathbf{x}^{(2)} + (1 - \alpha)\mathbf{x}^{(1)}$ also belong to $S$. This will happen if all the inequality constraints are convex and all the equality constraints are linear. If an equality constraint is nonlinear, then it is curved, and if we connect two points on the line by a straight segment, the interior of the segment will not satisfy the equality constraint, and this will violate the convexity requirement. Figure 4-9(b) shows examples of a convex set, while Figure 4-9(c) shows an example of a non-convex set. When the feasible set is convex and the objective function is convex, the optimization problem is called a convex problem. For a convex problem, a local minimum is also a global minimum.

## 4.4. Optimality criteria

Once an optimization problem is formulated, it is often solved using numerical optimization techniques, which will be discussed in Chapters 5 and 6. If the graph of the objective function over the entire feasible set is known, it would be possible to find the optimum design graphically. However, this information is barely available for most applications, especially for high-dimensional design problems. Therefore, most optimization algorithms try to find the optimum design by moving from one design to another iteratively. In such an iterative process, it would be necessary to determine if a new design is optimum or not. Optimality criteria are conditions that an optimum design must satisfy. Optimality criteria are considered one of the most important concepts in design optimization. Therefore, it would be important to fully understand them.

*Global versus local optimum*

Before discussing optimality criteria, it would be necessary to understand the local and global optima. The global optimum is the design that has the lowest value of objective function within the feasible set. The goal of an optimization problem is to find the global optimum. The issue related to the global optimum is that it is difficult to find it. For most engineering applications, the functional form of the objective function is usually unknown. Optimization algorithms iteratively improve the current design by moving to a new design that has a lower objective function. If there is no way to lower the objective function from the current design, this design should satisfy optimality criteria. However, even if the current design is the optimum design in the immediate neighborhood, it does not mean that it is the best design in the entire feasible set. Figure 4-10 shows an illustration of an objective function as a function of a design variable. The yellow circles represent local optima, which are the best designs in the immediate neighborhood. The red circle is indeed the global optimum design, which has the lowest value of the objective function in the feasible set. If an optimization algorithm starts from different designs, it is possible that it may find different local optima or a global optimum. The challenge is that it is difficult to determine if the optimum design that is found by an optimization algorithm is a local or global optimum.

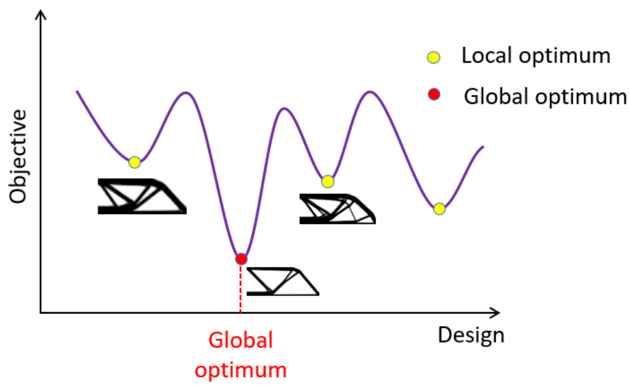


Figure 4-10: Global versus local optima.

Mathematically, a design $\mathbf{x}^*$ is called a global optimum for $f(\mathbf{x})$ if

$$f(\mathbf{x}^*) \leq f(\mathbf{x}), \qquad \text{for all } \mathbf{x} \in S \tag{4.9}$$

where $S$ is the feasible set that satisfies all constraints. The practical difficulty associated with the global optimum is that there is no mathematical method to find it. However, the existence of the global optimum can be provided by the Weierstrass theorem or the extreme value theorem [42]: If $f(\mathbf{x})$ is continuous and the feasible set $S$ is closed and bounded, then there is a global minimum. The unbounded feasible set was graphically illustrated in Figure 4-5(a). A bounded set means that the area (or volume in 3D or hyper-volume in high dimension) that is covered by the feasible set is finite. The closed set means that the inequality constraints are in the form of less-than-or-equal-to ($\leq$) so that the constraint boundary is included in the feasible set.

A design $\mathbf{x}^*$ is called a local optimum for $f(\mathbf{x})$ if

$$f(\mathbf{x}^*) \leq f(\mathbf{x}), \qquad \text{for all } \mathbf{x} \in S \text{ in a small neighborhood of } \mathbf{x}^* \tag{4.10}$$

In Figure 4-10, all yellow circles are local optima where they are the lowest points in a small neighborhood. Since it is impractical to search the entire feasible set, almost all numerical optimization algorithms can only guarantee a local optimum, not the global one.

*Unconstrained optimization*

In order to develop the optimality criteria, the local and global optimal shown in Figure 4-10 give a clue. Both the local and global optima have their extreme value, where the slope becomes zero. That is, at optimum the function may satisfy $\mathrm{d}f(x)/\mathrm{d}x = 0$; that is, the design is at a stationary point or an extreme value. However, this cannot be generalized for arbitrary functions. Figure 4-11(a) shows two functions $f_1(x) = |x - 5|$ and $f_2(x) = 0.2(\mathrm{x} - 5)^2$. Both functions have the global optimum at $x = 5$. However, $\mathrm{d}f_1(x)/\mathrm{d}x \neq 0$ at $x = 5$. In fact, $\mathrm{d}f_1(x)/\mathrm{d}x$ cannot be defined at $x = 5$. This is because $f_1(x)$ is not a smooth function of $x$ and non-differentiable. Therefore, optimality criteria assume that the function is smooth with respect to design variables.

Even if a function is smooth, the condition of $\mathrm{d}f(x)/\mathrm{d}x = 0$ is not enough to determine if a design $x$ is optimum or not. Figure 4-11(b) shows three functions. All three functions have $\mathrm{d}f(x)/\mathrm{d}x = 0$ at $x =$

5. Among the three, however, only $f(x) = (x-5)^2$ has a minimum at $x = 5$. The other function $f(x) = 10x - x^2$ has its maximum, and $f(x) = 0.2(x-5)^3$ has no minimum or maximum at $x = 5$. In fact, this point is an inflection point. In optimization theory, the requirement of $\mathrm{d}f(x)/\mathrm{d}x = 0$ is called a necessary condition. If a design is optimum, it must satisfy the necessary condition. However, not all designs that satisfy the necessary condition are optimum.

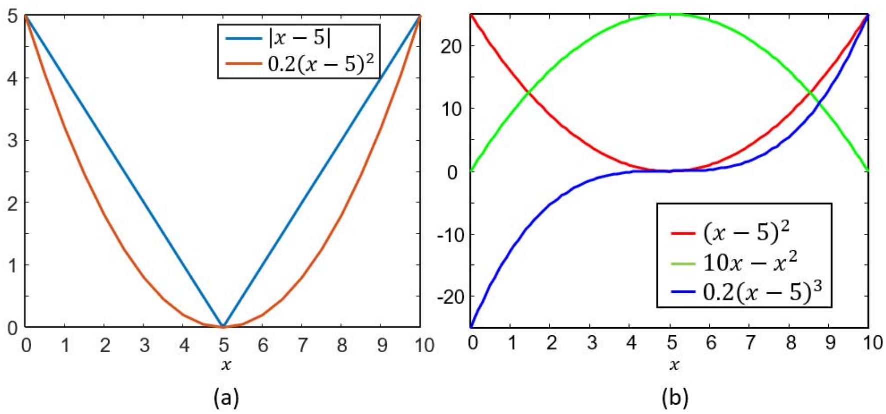


Figure 4-11: Optimum design of a smooth and non-smooth function.

Consider the following unconstrained optimization problem with a single variable:

$$\underset{x}{\text{minimize}}\, f(x) \tag{4.11}$$

If $x^*$ is a local minimum, for an arbitrary neighboring point $x = x^* + \Delta x$, the function must satisfy $f(x) \geq f(x^*)$. Using the Taylor series expansion, the function $f(x)$ can be expanded with respect to $f(x^*)$ as

$$f(x) = f(x^* + \Delta x) = f(x^*) + f'(x^*)\Delta x + \tfrac{1}{2} f''(x^*)\Delta x^2 + \mathrm{H.O.T.}$$

where $\mathrm{H.O.T.}$ represents high-order terms, and $f'$ and $f''$ are respectively the first- and second-order derivatives. If $f(x^*)$ is a local minimum, then the following functional difference must be non-negative:

$$\Delta f = f(x) - f(x^*) = f'(x^*)\Delta x + \tfrac{1}{2} f''(x^*)\Delta x^2 + \mathrm{H.O.T.} \tag{4.12}$$

For $x^*$ to be a local minimum, it would be necessary that $\Delta f \geq 0$. Assuming $\Delta x$ is small, the term including $\Delta x^2$ and higher-order terms can be ignored. Therefore, $\Delta f \approx f'(x^*)\Delta x \geq 0$ for arbitrary $\Delta x$. The only possibility that this inequality satisfies for arbitrary $\Delta x$ is that its coefficient $f'(x^*)$ must vanish. Otherwise, $\Delta f$ can be negative if $-\Delta x$ is used instead. Therefore, from this argument, it is possible to obtain the following first-order necessary condition of optimum design:

$$f'(x^*) \equiv \frac{df(x^*)}{dx} = 0 \tag{4.13}$$

This seemingly obvious condition is called Karush-Kuhn-Tucker (KKT) condition [43, 44], which is the most popular condition in optimum design.

Once $f'(x^*) = 0$ is satisfied, Eq. (4.12) becomes

$$\Delta f = \tfrac{1}{2} f''(x^*)\Delta x^2 + \mathrm{H.O.T.} \geq 0 \tag{4.14}$$

Since $\Delta x^2 > 0$ always, the second-order necessary condition would be

$$f''(x^*) \equiv \frac{d^2 f(x^*)}{dx^2} \geq 0 \tag{4.15}$$

Therefore, if a design $x^*$ is a local optimum, Eqs. (4.13) and (4.15) must satisfy. That is, they are first- and second-order necessary conditions. On the other hand, the sufficient condition is given as

$$f'(x^*) = 0 \text{ and } f''(x^*) > 0 \tag{4.16}$$

The positiveness of the second-order derivative is an important property of a function. This is indeed the Hessian information in Eq. (4.8). The positive second-order derivative is equivalent to the positive definite matrix for a multi-variable function. Therefore, it is related to the convexity of a function. The curvature of a function is related to the second-order derivative. That is, the curvature $\kappa(x)$ can be defined by $\kappa(x) = f''(x)/(1 + f'^2)^{1.5}$. Geometrically this makes sense as a function with a positive curvature has a minimum point.

**Example 4-7**

Consider a polynomial function $f(x) = x^3 - 3x$ in the design space $x \in [-2,2]$. Classify the stationary points of the function from the optimality criteria and check by plotting them.

**Solution**:

Since optimum designs must satisfy the KKT condition, it makes sense to find $x$ where the gradient vanishes.

$$f'(x) = 3x^2 - 3 = 0 \quad \rightarrow \quad x = -1 \text{ or } x = 1$$

That means both $x = -1$ and $x = 1$ are candidate points for optima. At $x = -1$, the second-order necessary condition $f''(x) = 6x = -6 < 0$ does not satisfy. In fact, this is the maximum point A as shown in Figure 4-12. The function has a maximum value $f(-1) = 2$ at point A. At $x = 1$, $f''(x) = 6x = 6 > 0$; that is the second-order necessary condition and sufficient condition are satisfied. Indeed, this is the minimum point B as shown in Figure 4-12.

In this particular problem, it is interesting to note that point C in Figure 4-12 is also a minimum point, while point D is a maximum point. However, these points do not satisfy both the necessary and sufficient conditions. This is because they are on the constraint bound. The optimality conditions with constraints will be discussed in the next subsection.

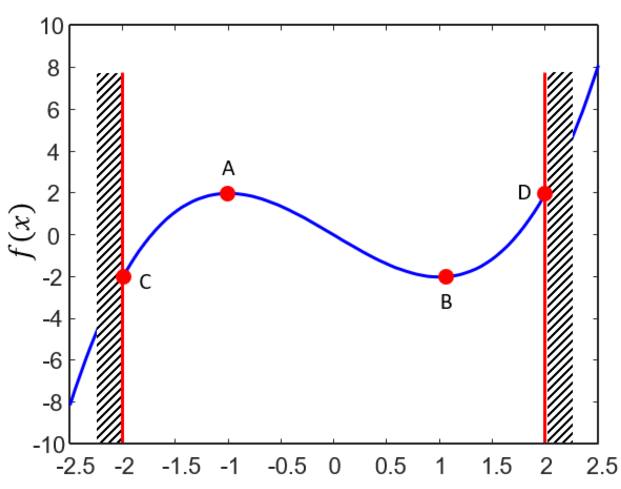


Figure 4-12: Optimum points of a cubic function with design space $x \in [-2,2]$.

The optimality criteria for a single-variable optimization problem can be extended to multi-variable optimization problems. Let the multi-dimensional design variables be defined as $\mathbf{x} = \{x_1, x_2, \cdots, x_n\}^T$. Let $\mathbf{x}^*$ be the optimum design and $\mathbf{x} = \mathbf{x}^* + \Delta\mathbf{x}$ be an arbitrary neighborhood. Then the Taylor series can be used to expand the objective function $f(\mathbf{x})$ with respect to $f(\mathbf{x}^*)$ as

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{x}^*) + \sum_{i=1}^{n} \frac{\partial f(\mathbf{x}^*)}{\partial x_i} \Delta x_i + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 f(\mathbf{x}^*)}{\partial x_i \partial x_j} \Delta x_i \Delta x_j + \text{H.O.T.} \\ &= f(\mathbf{x}^*) + \Delta\mathbf{x}^T \nabla f(\mathbf{x}^*) + \frac{1}{2} \Delta\mathbf{x}^T \mathbf{H}(\mathbf{x}^*) \Delta\mathbf{x} + \text{H.O.T.} \end{aligned} \tag{4.17}$$

where $\nabla f(\mathbf{x}^*)$ is the vector of gradients in Eq. (4.7) and $\mathbf{H}(\mathbf{x}) = \nabla^2 f(\mathbf{x})$ is the Hessian matrix defined in Eq. (4.8).

In order to satisfy $\Delta f = f(\mathbf{x}) - f(\mathbf{x}^*) \geq 0$ for arbitrary $\mathbf{x}$ in the neighborhood of $\mathbf{x}^*$, it would be necessary that $\nabla f(\mathbf{x}^*) = 0$. If $\partial f / \partial x_i \neq 0$, it is possible to choose $(x_i - x_i^*)$ in the opposite direction and other $(x_j - x_j^*) = 0$ to make $\Delta f < 0$. Therefore, in order to satisfy $f(\mathbf{x}^*)$ being the minimum, it would be necessary that $f(\mathbf{x}^*)$ needs to be stationary; that is, $\nabla f(\mathbf{x}^*) = 0$.

Now with $\nabla f(\mathbf{x}^*) = 0$, the change of the objective function becomes $\Delta f = \frac{1}{2} \Delta\mathbf{x}^T \mathbf{H}(\mathbf{x}^*) \Delta\mathbf{x} + \text{H.O.T.}$ Therefore, the sufficient condition for $f(\mathbf{x}^*)$ being the minimum is that

$$\Delta\mathbf{x}^T \mathbf{H}(\mathbf{x}^*) \Delta\mathbf{x} > 0 \text{ for all } \Delta\mathbf{x} \neq 0 \tag{4.18}$$

This means that the matrix of second-order derivatives (Hessian) is positive definite. In the same argument in Eq. (4.15), the second-order necessary condition would satisfy if the Hessian matrix is positive semi-definite. It would be impractical to check the positive definiteness for all $\Delta\mathbf{x} \neq 0$. Instead, the simplest way to check positive definiteness is to check if all eigenvalues of the Hessian matrix are positive. On the other hand, if the Hessian matrix is positive semi-definite, then it is the second-order necessary condition. The eigenvalues of the positive semi-definite matrix are non-negative.

In summary, the following optimality criteria can be summarized for multi-variable optimization problems:

KKT condition
$$\nabla f(\mathbf{x}^*) = 0 \tag{4.19}$$

2nd-order necessary condition
$$\Delta\mathbf{x}^T \mathbf{H}(\mathbf{x}^*) \Delta\mathbf{x} \geq 0 \text{ for all } \Delta\mathbf{x} \neq 0 \tag{4.20}$$

Sufficient condition
$$\Delta\mathbf{x}^T \mathbf{H}(\mathbf{x}^*) \Delta\mathbf{x} > 0 \text{ for all } \Delta\mathbf{x} \neq 0 \tag{4.21}$$

The positive definite matrix in Eq. (4.21) is indeed a quadratic form defined as $q = \Delta\mathbf{x}^T \mathbf{H}(\mathbf{x}^*) \Delta\mathbf{x}$. Assuming that the KKT condition is satisfied, the minimum or maximum of the function can be determined by the property of the quadratic form. The following table summarizes them:

| Quadratic form | Hessian matrix | Extreme |
|---|---|---|
| $q > 0$ | Positive definite | Minimum |
| $q \geq 0$ | Positive semi-definite | Possibly minimum |
| $q < 0$ | Negative definite | Maximum |
| $q \leq 0$ | Negative semi-definite | Possibly maximum |
| $q \geq 0$ or $q \leq 0$ | Indefinite | Saddle point |

**Example 4-8**

Find a stationary point of the following objective functions and determine if the stationary point is minimum, maximum, or saddle point: (a) $f_1(x_1, x_2) = x_1^2 + x_1x_2 + x_2^2$ and (b) $f_2(x_1, x_2) = x_1^2 + 3x_1x_2 + x_2^2$.

**Solution**:
(a) For, $f_1(x_1, x_2) = x_1^2 + x_1x_2 + x_2^2$, the stationary points can be found using the KKT condition as

$$\nabla f_1 = \begin{Bmatrix} 2x_1 + x_2 \\ x_1 + 2x_2 \end{Bmatrix} = 0$$

By solving the system of equations, the stationary point turns out to be $\{x_1, x_2\} = \{0, 0\}$. At this stationary point, the Hessian matrix becomes

$$\mathbf{H} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

The eigenvalue of the Hessian matrix can be obtained by solving $|\mathbf{H} - \lambda\mathbf{I}| = 0$, where **I** is the identity matrix. The eigenvalues that make the determinant zero are $\lambda_1 = 1$ and $\lambda_2 = 3$. Since both eigenvalues are positive, the Hessian matrix is positive definite, and the stationary point $\{x_1, x_2\} = \{0, 0\}$ satisfies sufficient condition; i.e., it is a minimum point. Figure 4-13(a) shows the plot of $f_1$, which confirms that it is the global minimum.

(b) For, $f_2(x_1, x_2) = x_1^2 + 3x_1x_2 + x_2^2$, the stationary points can be found using the KKT condition as

$$\nabla f_2 = \begin{Bmatrix} 2x_1 + 3x_2 \\ 3x_1 + 2x_2 \end{Bmatrix} = 0$$

By solving the system of equations, the stationary point turns out to be $\{x_1, x_2\} = \{0, 0\}$. At this stationary point, the Hessian matrix becomes

$$\mathbf{H} = \begin{bmatrix} 2 & 3 \\ 3 & 2 \end{bmatrix}$$

The eigenvalues that make the determinant zero are $\lambda_1 = -1$ and $\lambda_2 = 5$. Since one eigenvalue is negative, while the other is positive, this stationary point is not a minimum or a maximum. In fact, this point is a saddle point as shown in Figure 4-13 (b). It is interesting to note that the saddle point is a minimum along the line $x_1 = x_2$, while it is a maximum along the line $x_1 = -x_2$.

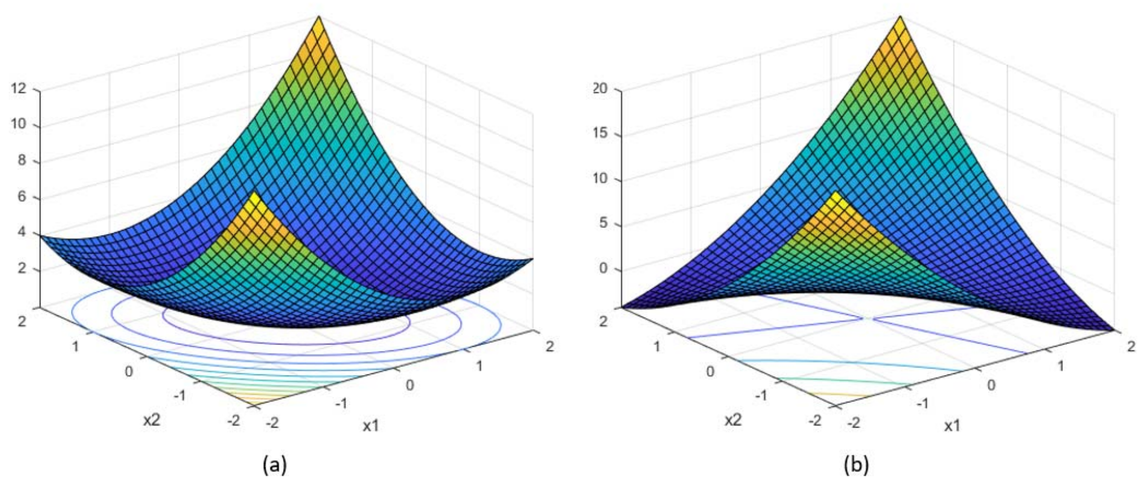


Figure 4-13: Surface plots of two functions in **Example 4-8**.

*Constrained optimization*

The necessary and sufficient conditions in the previous section are purely determined by the objective function because there was no constraint. However, as shown in **Example 4-7**, the two points C and D do not satisfy the optimality criteria but they were a minimum and a maximum point because of constraints. Therefore, it is obvious that constraints play an important role in optimality criteria. Before we formally develop optimality criteria for a constrained optimization problem, it would be beneficial to investigate the effect of constraints for optimum design. The following examples can provide useful insights into constrained optimization.

**Example 4-9**

First, let us consider the following optimization problem with an inequality constraint:

$$\begin{aligned} &\text{minimize } \ f(\mathbf{x}) = (x_1 - 1)^2 + (x_2 - 1)^2 \\ &\text{subject to } g(\mathbf{x}) = x_1 + x_2 - 4 \le 0 \end{aligned}$$

The stationary point for the objective function can be obtained from

$$\nabla f = \begin{Bmatrix} 2(x_1 - 1) \\ 2(x_2 - 1) \end{Bmatrix} = 0$$

which can be solved for $\{x_1, x_2\} = \{1, 1\}$. The Hessian matrix at this point is $\mathbf{H} = 2\mathbf{I}$, which is positive definite. Also, at this point, the inequality constraint $g(\mathbf{x}) = x_1 + x_2 - 4 = -2 < 0$. Since this point satisfies the inequality, this point is an optimum point. As shown in Figure 4-14(a), the objective function has its minimum $f^* = 0$ at $\{x_1, x_2\} = \{1, 1\}$, and it belongs to the feasible domain. In this case, the constraint does not play any role in optimum design. In general, when an optimum design is inside of the feasible domain, the constraint is inactive and does not play any role in optimum design.

As a second example, let us consider a different objective function but with the same inequality constraint:

$$\begin{aligned} &\text{minimize } \ f(\mathbf{x}) = (x_1 - 3)^2 + (x_2 - 3)^2 \\ &\text{subject to } g(\mathbf{x}) = x_1 + x_2 - 4 \le 0 \end{aligned}$$

In this case, the stationary point of the objective function is at $\{x_1, x_2\} = \{3, 3\}$, and the Hessian is also positive definite. However, the inequality constraint $g(\mathbf{x}) = x_1 + x_2 - 4 = 2 > 0$ is violated at this point. Therefore, this point cannot be an optimum design. As shown in Figure 4-14(b), the stationary point is out of the feasible domain. The concentric circles in the figure are the contour of the objective function. The objective function has its minimum at $\{x_1, x_2\} = \{3, 3\}$ and gradually increases until it meets a point $\{x_1, x_2\} = \{2,2\}$, where it is the lowest objective function while satisfying the inequality constraint. Therefore, this is an optimum point, although the gradient of the objective function $\nabla f \neq 0$. In this case, the inequality constraint is active and plays a critical role in determining the objective function. The optimum design is located on the boundary of the feasible domain. When an inequality constraint is active, it becomes equality; that is, $g(\mathbf{x}) = x_1 + x_2 - 4 = 0$.

Lastly, let us consider the same objective function with an equality constraint:

$$\begin{aligned} &\text{minimize } \ f(\mathbf{x}) = (x_1 - 1)^2 + (x_2 - 1)^2 \\ &\text{subject to } g(\mathbf{x}) = x_1 + x_2 - 4 = 0 \end{aligned} \tag{4.22}$$

Different from inequality constraints, an equality constraint is always active. As shown in Figure 4-14(c), the feasible domain is the line of constraint $g(\mathbf{x}) = x_1 + x_2 - 4 = 0$. The contour of the objective function meets with the feasible set at $\{x_1, x_2\} = \{2,2\}$ first time, which is the optimum design. An equality constraint is always active, and the optimum design is located on the constraint boundary.

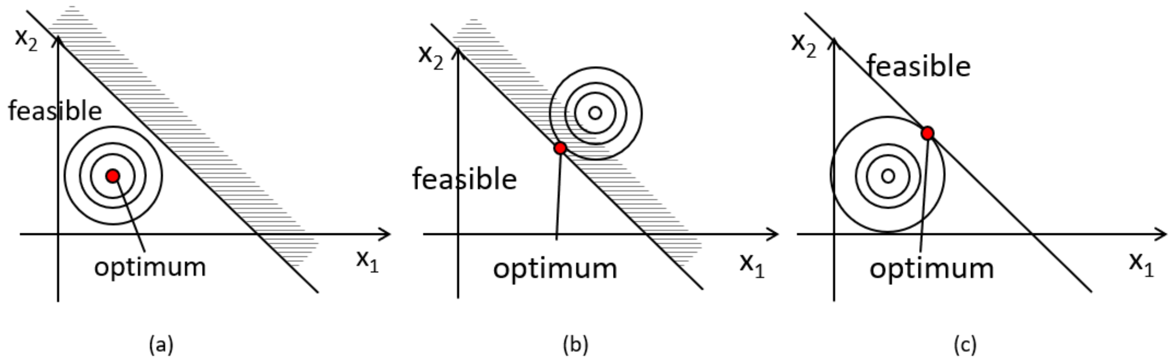


Figure 4-14: The effect of constraints on optimum design.

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It is interesting to note that an equality constraint can reduce the number of design variables. In the previous example, the relationship between the two design variables can be obtained using the equality constraint; that is, $x_2 = 4 - x_1$. If this relationship is used to remove variable $x_2$ from the objective function, the original constrained optimization problem becomes unconstraint one $f(x_1) = (x_1 - 1)^2 + (3 - x_1)^2$ with a single design variable. In general, it may not be possible to reduce design variables explicitly because an equality constraint can be an implicit function of design variables. However, its effect should be the same as reducing design variables.

In the previous example, if an additional equality constraint exists, then the optimum design is nothing but the intersection of the two equality constraints because that is the only feasible point. This is basically the same as two equations in a two-dimensional domain, where a unique solution is expected. If there are three independent equality constraints, then the problem is overly constrained and does not have a solution. Therefore, the number of equality constraints should be less than the number of design variables. Considering the fact that an active inequality constraint plays the same role as an equality constraint, the total number of active inequality constraints and equality constraints should be less than the number of design variables.

Now, optimality criteria for a general constrained optimization problem are presented. First, only a single equality constraint is considered. Consider the following constrained optimization problem with an equality constraint:

$$\begin{aligned} &\text{minimize } \ f(\mathbf{x}) \\ &\text{subject to } h(\mathbf{x}) = 0 \end{aligned} \tag{4.23}$$

Instead of solving the constrained optimization problem, it is converted into an unconstrained optimization problem by using the Lagrange multiplier method. That is, the constrained optimization problem in Eq. (4.23) is equivalent to the following unconstrained optimization problem:

$$\text{minimize } \ L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda h(\mathbf{x}) \tag{4.24}$$

where $\lambda$ is the Lagrange multiplier and $L(\mathbf{x}, \lambda)$ is referred to as the Lagrangian function. That is, the objective and constraint functions are linearly combined using the Lagrange multiplier. The main difference is that an additional variable $\lambda$ is introduced in addition to design variables $\mathbf{x}$.

Then, the necessary conditions for the stationary Lagrangian function are that the derivatives with respect to the design variables and the Lagrange multiplier are zero. That is,

$$\nabla L(\mathbf{x},\lambda)=0\ \rightarrow\ \begin{cases}\dfrac{\partial f(\mathbf{x})}{\partial \mathbf{x}}+\lambda\dfrac{\partial h(\mathbf{x})}{\partial \mathbf{x}}=0\\ h(\mathbf{x})=0\end{cases} \tag{4.25}$$

Therefore, in the case of a constrained optimization problem, the necessary conditions do not require the stationary condition of the objective function: $\nabla f \neq 0$. Instead, the linear combination of the gradient of the objective function and that of the constraint, scaled by the Lagrange multiplier, vanishes. Also, the equality constraint must satisfy at the optimum point. Because of the relation $\nabla f(\mathbf{x}) = -\lambda\nabla h(\mathbf{x})$, the Lagrange multiplier is often called "shadow prices", which means the price of constraints. If $\nabla h(\mathbf{x})$ is small, a large value of $\lambda$ is required to equilibrate it with the gradient of the objective function.

The KKT condition in Eq. (4.25) is for a single equality constraint. There are $n+1$ variables, and Eq. (4.25) provides $n+1$ equations. For a general optimization problem with $M$ equality constraints, we need the same number of Lagrange multiplier. Therefore, the equivalent unconstrained optimization problem can be written as

$$\text{minimize}\ \ L(\mathbf{x},\boldsymbol{\lambda})=f(\mathbf{x})+\sum_{j=1}^{M}\lambda_j h_j(\mathbf{x}) \tag{4.26}$$

where $\boldsymbol{\lambda}=\{\lambda_1,\lambda_2,\cdots,\lambda_M\}^T$ is the vector of Lagrange multipliers. Each constraint has a Lagrange multiplier. The KKT condition becomes

$$\nabla L(\mathbf{x},\boldsymbol{\lambda})=0\ \rightarrow\ \begin{cases}\dfrac{\partial f(\mathbf{x})}{\partial \mathbf{x}}+\displaystyle\sum_{j=1}^{M}\lambda_j\dfrac{\partial h_j(\mathbf{x})}{\partial \mathbf{x}}=0\\ h_j(\mathbf{x})=0, \qquad j=1,\cdots,M\end{cases} \tag{4.27}$$

The above KKT conditions have $n+M$ variables and $n+M$ equations.

**Example 4-10**

Find an optimum point that satisfies the KKT condition for the equality constraint in **Example 4-9**.

**Solution**:

For the constrained optimization problem in Eq. (4.22), the Lagrangian function can be defined as

$$L(\mathbf{x},\lambda)=(x_1-1)^2+(x_2-1)^2+\lambda(x_1+x_2-4)$$

The KKT condition is the stationary condition of the Lagrangian function as

$$\frac{\partial L}{\partial x_1}=2(x_1-1)+\lambda=0$$
$$\frac{\partial L}{\partial x_2}=2(x_2-1)+\lambda=0$$
$$\frac{\partial L}{\partial \lambda}=x_1+x_2-4=0$$

The above three equations can be solved for $\{x_1,x_2\}=\{2,2\}$, and $\lambda=-2$.

---

**Example 4-11**

Consider a quadratic objective function and a quadratic constraint that requires the design to be on a circle with a radius of 10 and a center at the origin. Find the points that satisfy the KKT condition and determine if they are minimum or maximum.

$$\begin{aligned} &\text{minimize } f(\mathbf{x}) = x_1^2 + 10x_2^2 \\ &\text{subject to } h(\mathbf{x}) = 100 - (x_1^2 + x_2^2) = 0 \end{aligned} \tag{4.28}$$

**Solution**:
Since the objective function prefers $x_1$ to $x_2$, the minimum may be expected for high $x_1$ and low $x_2$. The Lagrangian function is defined as

$$L(\mathbf{x}, \lambda) = x_1^2 + 10x_2^2 + \lambda(100 - x_1^2 - x_2^2)$$

Taking derivatives with respect to $x_1$, $x_2$, and $\lambda$, we get three equations, with the last being the constraint equations.

$$\frac{\partial L}{\partial x_1} = 2x_1 - 2\lambda x_1 = 0$$
$$\frac{\partial L}{\partial x_2} = 20x_2 - 2\lambda x_2 = 0$$
$$\frac{\partial L}{\partial \lambda} = 100 - x_1^2 - x_2^2 = 0$$

The first two equations will produce contradictory values for $\lambda$ if both $x_1$ and $x_2$ are non-zero. That indicates that a minimum will be obtained when $x_2 = 0$ and a maximum when $x_1 = 0$. Since all the terms are quadratic, we can change the sign of $x_1$ or $x_2$ without changing the results. These correspond to moving 180-deg around the circle. Then, we have four points that satisfy the KKT conditions:

$$x_1 = 0, x_2 = \pm 10 \ (f = 1{,}000, \text{maxima})$$
$$x_1 = \pm 10, x_2 = 0 \ (f = 100, \text{minima})$$

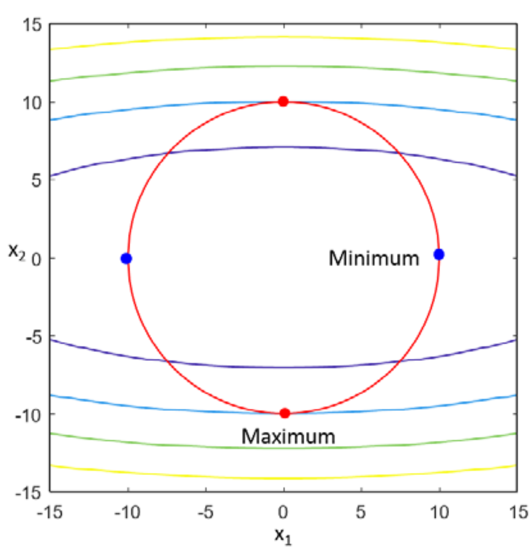

Figure 4-15: Maxima and minima of a quadratic objective function with a quadratic constraint.

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The optimality criteria for inequality constraint are based on the fact that when the inequality constraint is inactive, it does not play a role in the optimum design, and when the inequality constraint is active, it is basically the same as an equality constraint in the previous subsection. Consider the following optimization problem with inequality constraints:

$$\begin{aligned}&\text{minimize } f(\mathbf{x})\\&\text{subject to } g_i(\mathbf{x}) \le 0, i = 1, \cdots, K\end{aligned} \tag{4.29}$$

Since we have KKT conditions for equality constraints, we can convert the inequality constraints to equality ones by adding a slack variable. That is,

$$g_i(\mathbf{x}) \le 0 \rightarrow \;\; g_i(\mathbf{x}) + s_i^2 = 0 \tag{4.30}$$

where $s_i^2 \ge 0$ is the slack variable. Therefore, an inequality constraint introduces an additional variable to the system. When the slack variable $s_i^2 = 0$, the inequality constraint becomes equality and active. When the slack variable is positive $s_i^2 > 0$, the constraint is inactive. When the slack variable is negative, $s_i^2 < 0$, it means that the constraint is violated.

After converting inequality constraints to equality ones, we use the same Lagrangian function to make an unconstrained optimization problem, as

$$\text{minimize } L(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{s}) = f(\mathbf{x}) + \sum_{i=1}^{K} \lambda_i (g_i(\mathbf{x}) + s_i^2) \tag{4.31}$$

The Lagrangian is a function of $n$ design variables, $K$ Lagrange multiplier, $K$ slack variables. Therefore, the stationary condition of the Lagrangian function will produce $n + 2K$ numbers of equations. The KKT condition becomes

$$\nabla L(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{s}) = 0 \;\rightarrow\; \begin{cases} \dfrac{\partial f(\mathbf{x})}{\partial \mathbf{x}} + \displaystyle\sum_{i=1}^{K} \lambda_i \dfrac{\partial g_i(\mathbf{x})}{\partial \mathbf{x}} = 0 \\ g_i(\mathbf{x}) + s_i^2 = 0, \qquad i = 1, \cdots, K \\ 2\lambda_i s_i = 0, \qquad i = 1, \cdots, K \end{cases} \tag{4.32}$$

The last $K$ equations, $\lambda_i s_i = 0$, is called complementary slackness or switching condition. This condition can be interpreted as $\lambda_i g_i = 0$ as $g_i = 0$ when $s_i = 0$. This condition implies that either the Lagrange multiplier is zero or the constraint is zero, which is why it is called complementary slackness. When the constraint is active, $g_i = 0$, the Lagrange multiplier is non-zero. If the constraint is inactive, it has a zero value. In particular, when the inequality constraint is less-than-or-equal-to type, the Lagrange multiplier of an active constraint becomes positive. Therefore, the complementary slackness can be summarized as

$$\begin{aligned}\lambda_i = 0 \;\rightarrow\; g_i < 0 \text{ inactive constraint}\\ \lambda_i > 0 \;\rightarrow\; g_i = 0 \text{ active constraint}\end{aligned} \tag{4.33}$$

This complementary slackness is consistent with the previous discussion that inactive constraints do not play any role in determining the optimum design. In Eq. (4.32), the summation in the first equation is only for active constraints because $\lambda_i$ for inactive constraints will be zero. It is noted that the Lagrange multiplier of an equality constraint can be either positive or negative.

**Example 4-12**

Find designs that satisfy the KKT conditions for the following constrained optimization problem:

$$\begin{aligned}&\text{minimize } f(\mathbf{x}) = (x_1 - 3)^2 + (x_2 - 3)^2\\&\text{subject to } h(x) = x_1 - 3x_2 - 1 = 0\\&\qquad\qquad g(\mathbf{x}) = x_1 + x_2 - 4 \le 0\end{aligned} \tag{4.34}$$

**Solution**:

The inequality constraint needs to introduce a slack variable. The Lagrangian function can be defined as

$$L(\mathbf{x}, \boldsymbol{\lambda}, s) = (x_1 - 3)^2 + (x_2 - 3)^2 + \lambda_1(x_1 - 3x_2 - 1) + \lambda_2(x_1 + x_2 - 4 + s^2)$$

The KKT conditions become

$$\nabla L(\mathbf{x}, \boldsymbol{\lambda}, s) = 0 \;\rightarrow\; \begin{cases} 2(x_1 - 3) + \lambda_1 + \lambda_2 = 0 \\ 2(x_2 - 3) - 3\lambda_1 + \lambda_2 = 0 \\ x_1 - 3x_2 - 1 = 0 \\ x_1 + x_2 - 4 + s^2 = 0 \\ s\lambda_2 = 0 \end{cases}$$

It is noted that all equations are linear, except for the complementary slackness term. Therefore, we can consider two cases separately: $\lambda_2 = 0$ or $s = 0$. Each case needs to satisfy all constraints.

Case 1) $\lambda_2 = 0$. In this case, the KKT conditions become

$$\begin{cases} 2(x_1 - 3) + \lambda_1 = 0 \\ 2(x_2 - 3) - 3\lambda_1 = 0 \\ x_1 - 3x_2 - 1 = 0 \\ x_1 + x_2 - 4 + s^2 = 0 \end{cases}$$

The above equations can be solved for $x_1 = 3.7$, $x_2 = 0.9$, $\lambda_1 = -1.4$, and $s^2 = -0.6$. The objective at this point is $f^* = 4.9$. Since it is required to be $s^2 \geq 0$, this condition violates the inequality condition.

Case 2) $s = 0$. In this case, the KKT conditions become

$$\begin{cases} 2(x_1 - 3) + \lambda_1 + \lambda_2 = 0 \\ 2(x_2 - 3) - 3\lambda_1 + \lambda_2 = 0 \\ x_1 - 3x_2 - 1 = 0 \\ x_1 + x_2 - 4 = 0 \end{cases}$$

The above equations can be solved for $x_1 = 3.25$, $x_2 = 0.75$, $\lambda_1 = -1.875$, and $\lambda_2 = 1.125 > 0$. The objective at this point is $f^* = 5.125$, which is larger than that of Case 1. Since the Lagrange multiplier of the inequality constraint is positive, this case is valid. Figure 4-16 shows the contour of the objective function along with the two constraints. Due to the equality constraint, the feasible domain is the blue-colored line. Case 2 is the point when both constraints are active, while Case 1 is the point where the inequality constraint is violated.

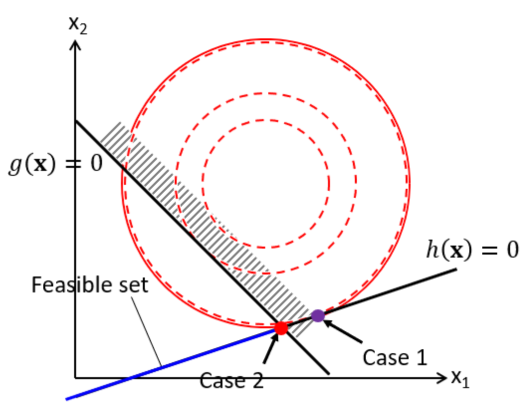


Figure 4-16: Objective and constraints of the optimization problem in **Example 4-12**.

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As shown in **Example 4-12**, the Lagrange multipliers play an important role in determining optimization. As mentioned before, the Lagrange multipliers are called “shadow prices”. This means how much constraint gradients need to change in order to compensate for the gradient of the objective function at the optimum design. From the first equation of the KKT condition in Eq. (4.32), the gradient of the objective function can be written as

$$\nabla_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{s}) = 0 \;\rightarrow\; \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = -\sum_{i=1}^{K} \lambda_i \frac{\partial g_i(\mathbf{x})}{\partial \mathbf{x}} \tag{4.35}$$

where $\nabla_{\mathbf{x}}$ means the derivative with respect to design variables $\mathbf{x}$. This relation means that the gradient of the objective function can be represented by a linear combination of active constraints. The Lagrange multipliers are the coefficients of each constraint gradient. As we discussed in the surrogate chapters, the coefficients represent the importance of the term. Therefore, the Lagrange multipliers represent how important the constraint is to compensate for the objective change. An inactive constraint would not contribute to the optimum design. An important constraint would contribute significantly to the objective change. At the optimum, as shown in Figure 4-17, the objective gradient can be represented by a linear combination of constraint gradients with Lagrange multipliers as a proportional constant.

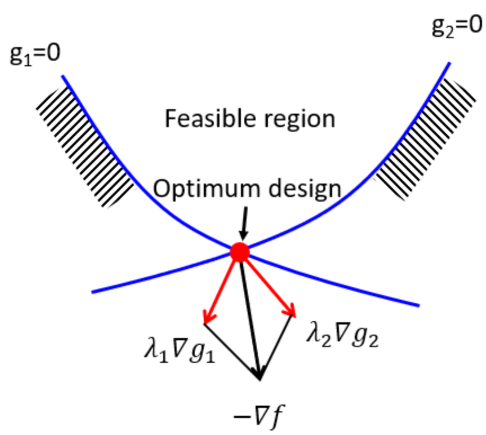


Figure 4-17: The relationship between objective gradient and constraint gradients at the optimum design.

The KKT conditions in Eq.(4.27) or Eq. (4.32) are necessary conditions; i.e., those points that satisfy the necessary conditions are the candidate for optimum design. Similar to the unconstrained optimization problem, it is possible to develop second-order necessary conditions and sufficient conditions. Consider the following general form of Lagrangian function:

$$\text{minimize } \; L(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{s}) = f(\mathbf{x}) + \sum_{j=1}^{M} \mu_j h_j(\mathbf{x}) + \sum_{i=1}^{K} \lambda_i \left(g_i(\mathbf{x}) + s_i^2\right) \tag{4.36}$$

where we used different notations for the Lagrange multipliers for the equality and inequality constraints. The first-order necessary condition in Eq.(4.27) or Eq. (4.32) can be represented by

$$\nabla L(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\lambda}, \mathbf{s}) = 0 \tag{4.37}$$

where the gradient operator is the derivative of all variables: $\nabla = \left\{\nabla_{\mathbf{x}}^T, \nabla_{\boldsymbol{\mu}}^T, \nabla_{\boldsymbol{\lambda}}^T, \nabla_{\mathbf{s}}^T\right\}^T$.

In the case of unconstrained optimization problems, the sufficient condition is that the Hessian matrix $\nabla^2 f$ is positive definite. In the case of constrained optimization problems, the sufficient condition that the Hessian of the Lagrangian function $\nabla_{\mathbf{xx}} L$ is positive definite in all feasible directions. A feasible direction is a direction in which a small change in the design keeps the design feasible. As shown in Figure 4-18, the optimum design is located on the boundary of active constraints. At this point, a feasible direction keeps the design in the feasible domain after a small movement in that direction. In the case of an equality constraint, the movement direction should be perpendicular to the gradient of the constraints. The gradient direction is the direction to change the constraint. Therefore, in order to keep the constraint satisfied after movement, the direction needs to satisfy $\nabla h_j \cdot \Delta\mathbf{x} = 0$. In the case of an inequality constraint, in order to make keep the constraint satisfied after movement, the direction needs to satisfy $\nabla g_i \cdot \Delta\mathbf{x} \leq 0$. However, the direction that makes $\nabla g_i \cdot \Delta\mathbf{x} < 0$ will make the constraint inactive after the movement. Therefore, in order to remain an active constraint, the inequality constraint also satisfy $\nabla g_i \cdot \Delta\mathbf{x} = 0$.

Therefore, the second-order necessary condition can be stated as

$$q = \Delta\mathbf{x}^T[\nabla_{\mathbf{xx}}L]\Delta\mathbf{x} \geq 0 \text{ for all } \Delta\mathbf{x} \neq 0 \text{ satisfying} \tag{4.38}$$

$$\begin{cases} \nabla g_i^T \Delta\mathbf{x} = 0 \text{ for all active inequalities} \\ \nabla h_j^T \Delta\mathbf{x} = 0 \text{ for all equalities} \end{cases} \tag{4.39}$$

In a similar way, the second-order sufficient condition can be stated as

$$q = \Delta\mathbf{x}^T[\nabla_{\mathbf{xx}}L]\Delta\mathbf{x} > 0 \text{ for all } \Delta\mathbf{x} \neq 0 \text{ satisfying Eq. (4.39)} \tag{4.40}$$

The feasible direction in Eq. (4.39) relaxes the requirement of positive definiteness of the Hessian matrix. It is enough that the Hessian matrix is positive definite only for feasible directions.

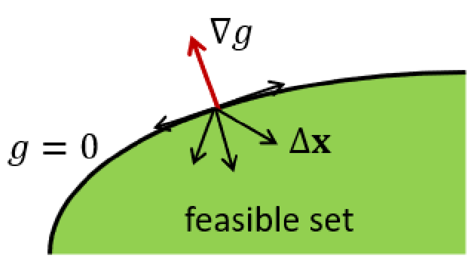


Figure 4-18: Constraint boundary and feasible direction.

*Effect of constraint limit*

In the previous subsection, it was shown that the Lagrange multipliers can be interpreted as "shadow prices" of constraint gradients in order to compensate for the gradient of the objective function at optimum design. There are different roles of the Lagrange multipliers in practical sense. The first important property of the Lagrange multipliers is that it can linearly approximate how much the optimum objective function will change when constraint bounds change.

Although the standard form of a constraint has a zero on the right-hand side, let us consider the constraint limit is on the right-hand side for this subsection. That is, the equality constraints are written as $h_i(\mathbf{x}) = a_i$, and the inequality constraints are written as $g_j(\mathbf{x}) \leq b_j$. Therefore, $a_i$ and $b_j$ are constraint limits. Then, if $a_i$ and $b_j$ change, the optimum design will also change. Therefore we can say that the optimum design is a function of these constraint bounds: $\mathbf{x}^* = \mathbf{x}^*(\mathbf{a}, \mathbf{b})$. If the optimum design changes, the objective function at the optimum design will also change: $f = f(\mathbf{a}, \mathbf{b})$. Then, the gradients of the objective function with respect to the constraint bounds are nothing but the negative of the Lagrange multipliers. In order to show this property, consider the following form of Lagrangian function:

$$L(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{s}) = f(\mathbf{x}, \mathbf{a}, \mathbf{b}) + \sum_{j=1}^{M} \mu_j(h_j(\mathbf{x}) - a_j) + \sum_{i=1}^{K} \lambda_i(g_i(\mathbf{x}) - b_i + s_i^2) \tag{4.41}$$

At the optimum design, the Lagrangian function needs to be stationary. Therefore, if the above equation is differentiated with respect to $a_j$ and $b_i$, we can obtain the following important results:

$$\frac{\partial f}{\partial a_j} = -\mu_j^*, \qquad \frac{\partial f}{\partial b_i} = -\lambda_i^* \tag{4.42}$$

where $\mu_j^*$ and $\lambda_i^*$ are Lagrange multipliers at the optimum design.

This information can be used to linearly approximate the change of optimum objective function due to the change in constraint bounds. For that purpose, we use the Taylor series expansion again. For a change of $a_j$ and $b_i$, the objective function at the optimum design can be expanded as

$$f^*(a_j + \Delta a_j, b_i + \Delta b_i) = f^*(a_j, b_i) + \frac{\partial f^*}{\partial a_j}\Delta a_j + \frac{\partial f^*}{\partial b_i}\Delta b_i + \text{H.O.T.} \tag{4.43}$$

Then, the change in the objective function can be estimated by

$$\Delta f^* = -\sum_{j=1}^{M} \mu_j^* \Delta a_j - \sum_{i=1}^{K} \lambda_i^* \Delta b_i \tag{4.44}$$

Therefore, when the constraint bounds are changed in a small amount, instead of solving the optimization problem again, it is possible to estimate how much the optimum objective function will change using Eq. (4.44).

Figure 4-19 shows how the change in the optimum design can be approximated using the Lagrange multiplier. The original optimum design is located at point A where both constraints are active: $g_1 = b_1$ and $g_2 = b_2$. When the constraint bound of $g_2$ is changed to $b_2 + \Delta b_2$, the true modified optimum design should be located at point B if the optimization problem is solved again with the new constraint bound. Instead, Eq. (4.44) can be used to approximate the change of the optimum objective function at point C. It is noted that Eq. (4.44) cannot approximate the new optimum design. It only approximates the change of the optimum objective function.

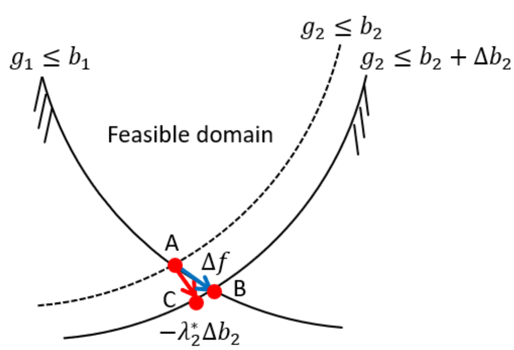


Figure 4-19: Change of the optimum objective function due to the change in constraint bound.

**Example 4-13**

Formulate an optimization problem to minimize the cost of building a top-open container box while the volume of the box should be greater than 125 $\text{ft}^3$. The side panel cost is $\$10/\text{ft}^2$, while the floor and ends panels are $\$15/\text{ft}^2$. The three design variables are the depth, length, and height of the box. (a) Formulate the optimization problem and solve it for the optimum design. (b) When the required volume increases to 130 $\text{ft}^3$, estimate the change in cost using the Lagrange multiplier. (c) Solve the optimization problem with the new constraint bound and compare the change in optimum objective function with that of (b).

**Solution**:

(a) Let design variables are $\{x_1, x_2, x_3\} = \{\text{depth}, \text{length}, \text{height}\}$. The optimization problem can be formulated as

$$\begin{aligned}&\text{minimize } f(\mathbf{x}) = 20x_2x_3 + 30x_1x_3 + 15x_1x_2 \\ &\text{subject to } g(\mathbf{x}) = 125 - x_1x_2x_3 \le 0\end{aligned}$$

The Lagrangian function is defined as

$$L(\mathbf{x}, \lambda, s) = 20x_2x_3 + 30x_1x_3 + 15x_1x_2 + \lambda(125 - x_1x_2x_3 + s^2)$$

The stationary condition of the Lagrangian function becomes

$$\nabla L(\mathbf{x}, \lambda, s) = 0 \ \rightarrow \ \begin{cases} 15x_2 + 30x_3 - \lambda x_2x_3 = 0 \\ 15x_1 + 20x_3 - \lambda x_1x_3 = 0 \\ 30x_1 + 20x_2 - \lambda x_1x_2 = 0 \\ 125 - x_1x_2x_3 + s^2 = 0 \\ s\lambda = 0 \end{cases}$$

The optimum design that satisfies the above KKT conditions is $x_1^* = 4.8075$, $x_2^* = 7.2112$, $x_3^* = 3.6056$. At the optimum design, the objective function and the Lagrange multiplier are $f^* = 1560$, $\lambda^* = 8.320$.

(b) When the constraint bound increases to $130 \text{ ft}^3$, its effect on the constraint bound changes from $-125$ to $-130$. This is because the constraint is written in standard form. Therefore, $\Delta b = -5$. The increase in the optimum objective function can be estimated by

$$\Delta f = -\lambda \Delta b = -8.320 \times -5 = 41.6$$

(c) The modified optimization problem is

$$\begin{aligned}&\text{minimize } f(\mathbf{x}) = 20x_2x_3 + 30x_1x_3 + 15x_1x_2 \\ &\text{subject to } g(\mathbf{x}) = 130 - x_1x_2x_3 \le 0\end{aligned}$$

The solution to the above optimization problem is $f^* = 1601.3$, where $\Delta f = 41.3$. Therefore, the approximation using the Lagrange multiplier ($\Delta f = 41.6$) is close to that of the actual change($\Delta f = 41.3$).

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*Sensitivity of optimum solution to parameters*

In optimization problems, design variables are the ones that can be changed by engineers to find an optimum design. However, most engineering applications have parameters, which are not design variables but they can be changed or the engineers want to see their effects on the optimum design. For example, when an engineering application includes frictional contact, the friction coefficient is uncontrollable but its exact value is difficult to identify. Therefore, engineers might want to see the effect of the friction coefficient on the optimum design. If the optimum objective is very sensitive to the friction coefficient, it would be necessary to identify it more carefully or use a conservative value to compensate for inaccurate information. As another example, Young's modulus is an important parameter for structural simulation. However, Young's modulus of steel has about 15% variability. Therefore, engineers may want to try different values of Young's modulus to understand its effect on the optimum design. Other common parameters are constraint bounds as we discussed in the previous subsection. In the case of a stress constraint, for example, $\sigma_{max} \le \sigma_{\text{limit}}$, where $\sigma_{\text{limit}}$ is an allowable strength of a material. In practice, since the allowable strength has uncertainty, we may want to get an estimate of how much the optimum objective will change if the allowable strength is increased by going to a better grade of material.

When an engineering application has uncontrollable parameters, it would be valuable to know the sensitivity (i.e., the gradient) of the optimum objective function with respect to the parameters. If the sensitivity is high, the parameter is important and needs to identify accurately or use a conservative value to compensate for its effect. If the sensitivity is low, the parameter will not have much effect on the optimum design. The Lagrange multipliers play an important role in this parameter sensitivity. In order to show it, it is assumed that the objective and constraints depend on a parameter $p$. For simplicity of presentation, we only consider the following optimization problem with an inequality constraint:

$$\begin{aligned} &\text{minimize } \ f(\mathbf{x}, p) \\ &\text{subject to } g(\mathbf{x}, p) \leq 0 \end{aligned} \tag{4.45}$$

More complicated optimization problems with equality and inequality constraints can be considered in a similar way. Since both objective and constraint depend on parameter $p$, it is obvious that the optimum design also depends on the parameter: $\mathbf{x}^*(p)$.

The objective function at the optimum design can be written as $f^*(p) = f(\mathbf{x}^*(p), p)$, as well as the constraint $g^*(p) = g(\mathbf{x}^*(p), p)$. Since the constraint is a function of both the parameter and the design variable, the sensitivity of the constraint with respect to the parameter can be written as

$$\frac{dg}{dp} = \frac{\partial g}{\partial p} + \frac{\partial g}{\partial \mathbf{x}}^T \frac{d\mathbf{x}}{\partial p} = 0 \tag{4.46}$$

where $dg/dp$ is the total derivative, while $\partial g/\partial p$ is the partial derivative. The second term on the right-hand side uses the chain rule of differentiation. The sensitivity of the objective function with respect to the parameter can be written in a similar form. By using Eqs. (4.35) and (4.46), the sensitivity of the objective function at the optimum design can be calculated as

$$\begin{aligned} \frac{df}{dp} &= \frac{\partial f}{\partial p} + \frac{\partial f}{\partial \mathbf{x}}^T \frac{d\mathbf{x}}{\partial p} \\ &= \frac{\partial f}{\partial p} - \lambda \frac{\partial g}{\partial \mathbf{x}}^T \frac{d\mathbf{x}}{\partial p} \\ &= \frac{\partial f}{\partial p} + \lambda \frac{\partial g}{\partial p} \end{aligned} \tag{4.47}$$

Equation (4.47) shows that the Lagrange multiplier is a measure of the effect of a change in the constraint on the objective function. Consider, for example, the constraint is given in the form of $g(\mathbf{x}) = G(\mathbf{x}) - p \leq 0$. By increasing $p$, we make the constraint easier to satisfy (i.e., stress limit is increased for stress constraint). If a constraint is relaxed, the optimum objective function can be reduced further. Since $\partial g/\partial p = -1$, from Eq. (4.47), $df/dp = -\lambda$. That is, the optimum objective function can be reduced by increasing $p$. In the opposite case (i.e., increasing a parameter makes the constraint more difficult to satisfy), $\lambda$ is the marginal price that we pay in terms of an increase in the objective function for making the constraint more difficult to satisfy.

There are two special cases that are worth noting. (a) When only the objective function depends on the parameter, it is remarkable that the total derivative is equal to the partial derivative. That means, that the effect of changing the optimum position $\mathbf{x}^*$ as a function of $p$ can be neglected. (b) When $p$ is the bound on a single constraint; that is, when the constraint can be written as $g(\mathbf{x}) = G(\mathbf{x}) - p \leq 0$, $df/dp = -\lambda$, which is why the Lagrange multipliers are called shadow prices.

**Example 4-14**

Consider the following optimization problem with an inequality constraint:

$$\text{subject to } g(\mathbf{x}, p) = p - (x_1^2 + x_2^2) \le 0$$

where $p$ is the square of the radius of the circle. (a) When $p = 100$, calculate the optimum design and optimum objective function along with the Lagrange multiplier. (b) Calculate the sensitivity of the optimum objective function with respect to the parameter $p$.

**Solution**:
The Lagrangian function and the KKT conditions can be written as

$$\text{minimize } L(\mathbf{x}, \boldsymbol{\lambda}, \mathbf{s}) = x_1^2 + 10x_2^2 + \lambda(p - x_1^2 - x_2^2 + s^2)$$

$$\nabla L(\mathbf{x}, \lambda, s) = 0 \ \rightarrow \begin{cases} 2x_1 - 2\lambda x_1 = 0 \\ 20x_2 - 2\lambda x_2 = 0 \\ p - x_1^2 - x_2^2 + s^2 = 0 \\ \lambda s = 0 \end{cases}$$

The above KKT conditions can be used to find the optimum design $x = \{\pm\sqrt{p}, 0\}$ where the objective function is $f^*(p) = p$, and its sensitivity is $df^*/dp = 1$. The sensitivity of the optimum objective function can also be calculated using Eq. (4.47) as

$$\frac{df}{dp} = \frac{\partial f}{\partial p} + \lambda \frac{\partial g}{\partial p} = 0 + 1 \times 1 = 1$$

This result can easily be verified since for any value of $p$ we get that the optimum is at $x_2^* = 0$ and $x_1^* = \pm\sqrt{p}$, so $f^*(p) = p$.

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## 4.5. Exercise

1. Formulate the optimization problem for each of the following problems. Identify design variables and objective function.
   (a) Find the aspect ratio of rectangle with the highest ratio of area to the square of the perimeter.
   (b) We need to fly to a city in Florida, rent a car, and visit Gainesville, Jacksonville, and Tampa and fly back from the last city you visit. What should your itinerary be to minimize your driving distance?
   (c) You need to perform a task once a month, on the same day of each month (e.g., the 13th). It is more inconvenient to do on a weekend. Select the day of the month to minimize the number of times it will fall on a weekend in one given year (not a leap year).
2. A rectangular underground storage tank is to be constructed and installed. Specifications require that the volume of the tank be $1000 \text{ m}^3$ and that the ratio of the lengths of any two sides is no greater than two. The top surface of the tank is to be 3 m below the ground surface when installed. The cost of construction of the tank is $\$150/\text{m}^2$ based on the surface area. Installation cost in the dollar is equal to 200 times the product of the area and the square of the depth of the hole to be excavated. For convenience, assume the tank and the hole cross-sectional area are the same, i.e., no clearance is required. Formulate the optimization problem to minimize the total project cost and write the result in standard form.
3. A coal mining company has three coal mines and four coal cellars. The company is trucking coal from three mines to four cellars before shipping out of the customer. To make efficient usage of trucks, the total delivery distance from mines to cellars by the trucks needs to be minimized. The following tables show that distance between three mines (Mine number 1, 2, and 3) and four cellars (Cellar number A, B, C, and D). Each truck can carry two tons of coal at one time. The amount of

coal produced at each coal mine and the amount of coal that can be stored at each cellar are given in the following table. Each delivery of the coal by truck means a round trip of the distance between the mine and cellar, since the truck will return empty to get more coal. Assume that the company has enough truck so each truck can move between a selected mine and cellar only. Formulate the problem in standard form. Do not normalize or attempt to solve. (Hint: There are 12 design variables).

| Mine number | Distance(meter) from Mine to Cellar | | | |
|---|---|---|---|---|
| | Cellar A | Cellar B | Cellar C | Cellar D |
| 1 | 3500 | 2900 | 3450 | 1290 |
| 2 | 1670 | 4500 | 2390 | 4230 |
| 3 | 2340 | 1250 | 2880 | 3770 |

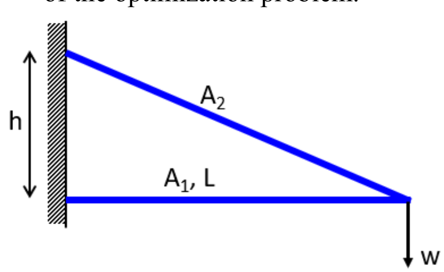
| Coal Production at Mines (per day) | |
|---|---|
| 1 | 3500 ton |
| 2 | 4000 ton |
| 3 | 4500 ton |

| Cellar Storage Capacity (per day) | |
|---|---|
| A | 2000 ton |
| B | 3000 ton |
| C | 4500 ton |
| D | 2500 ton |

4. Find the optimum design of the following optimization problem using graphical optimization.

$$\begin{aligned} \underset{x_1,x_2}{\text{minimize}} \quad & f = -x_1 - x_2 \\ \text{subject to} \quad & 2x_1 + 3x_2 \le 12 \\ & 2x_1 + x_2 \le 8 \\ & x_1, x_2 \ge 0 \end{aligned}$$

5. Solve **Example 4-5** when design variables are the outer radius $R_o$ and inner radius $R_i$.
6. A two-bar truss as shown in the figure is under a vertical load $W$. The goal of the optimization problem is to minimize the weight of the truss. The constraints are (a) each member stress should be less than the yield stress $\sigma_Y$, (b) the tip deflection should be less than the allowable displacement $u_{allowable}$, and (c) the compressive stress should be less than the buckling stress. When design variables are the two cross-sections, $A_1$ and $A_2$, the height $h$, and the length $L$, write the standard form of the optimization problem.




7. Provide two formulations in standard form for minimizing the surface area of a cylinder of a given volume when the diameter and height are the design variables. One formulation should use the volume as equality constraint, and another use it to reduce the number of design variables.
8. Formulate in standard form the problem of finding an open-top rectangle container with a volume of at least 50 and minimum surface area.
9. You need to go from point A to point B in minimum time while maintaining a safe distance from point C. Formulate an optimization problem in standard normalized form to find the path with no

more than three design variables when $A = (0,0), B = (10,10), C = (4,4)$, and the minimum safe distance is 5.

10. Check for the convexity of the following functions. If the function is not convex everywhere, check its domain of convexity.
(a) $f(x_1, x_2) = x_1^3 + 2x_2^2$
(b) $f(x_1, x_2) = 3x_1^2 + 2x_1x_2 + 2x_2^2 - 8$
(c) $f(x_1, x_2) = x_1^3 + 12x_1x_2^2 + 2x_2^2 + 5x_1^2$
11. Consider the following optimization of a quadratic objective function with a ring constraint

$$\underset{x_1,x_2}{\text{minimize}} \;\; f(x_1, x_2) = x_1^2 + 10x_2^2$$
$$\text{subject to} \;\; 81 \leq x_1^2 + x_2^2 \leq 1000$$

(a) Where is the minimum? What starting points (note the plural) will not find it when using fmincon? What is the problem preventing fmincon to reach the minimum?
(b) For the problem above, we found that the inner ring constraint was active, and its Lagrange multiplier was equal to 1. Calculate an estimate based on the Lagrange multiplier of the effect of changing the constraint from 81 to 79?
12. Classify the stationary points of the following functions from the optimality criteria, then check by plotting them. (a) $f(x) = 2x^3 + 3x^2$, (b) $f(x) = 3x^4 + 4x^3 - 12x^2$, (c) $f(x) = x^5$, and (d) $f(x) = x^4 + 4x^3 + 6x^2 + 4x$.
13. Find the stationary points of the following function and classify them: $f(x_1, x_2, x_3) = -x_1^2 + 2x_2x_3 + x_2^2 + 4x_3^2$.
14. The objective function $f = x_1 + 2x_2$ is to be minimized subject to the constraint that $x_2$ is larger than $-5$, and that the point is inside the circle $x_1^2 + x_2^2 = R^2$. (a) Write the Kuhn-Tucker conditions for the problem. (b) For $R^2 = 34$, check that the optimum is at $x_1 = -3, x_2 = -5$, and calculate the Lagrange multipliers. (c) Calculate the derivative of the optimum objective with respect to R, by using the Lagrange multipliers. (d) Use the equations for the derivatives of an optimum solution to obtain the derivatives of x and the Lagrange multiplier with respect to $R$. Use the results to check on (c). (e) Use the results to extrapolate the optimal solution for the largest value of $R$ for which you think that extrapolation makes sense. Explain.
15. The objective function $f = 3x_1 + 4x_2$ is to be minimized subject to the constraint that both $x_1$ and $x_2$ are less than 5 in magnitude, and that the point is inside the circle $x_1^2 + x_2^2 = R^2$. (a) Write the optimization problem in standard form. (b) For $R = 5$, check that the optimum is at $x_1 = -3, x_2 = -4$, and the Lagrange multiplier associated with the circle constraint is equal to 0.5. (c) Calculate the derivative of the optimum objective with respect to $R$, by using the Lagrange multiplier. (d) Use the equations for the derivatives of an optimum solution to obtain the derivatives of **x** and the Lagrange multiplier with respect to $R$. Use the results to check on (c). (e) Use the results to extrapolate the optimal solution for the largest value of $R$ for which you think that extrapolation makes sense. Explain.
16. Given the objective function $f = (x_1 + x_2)^2/x_1$, what is the error in the forward difference derivatives at that point if the increments in $x_1$ and $x_2$ are one percent of their value?
17. Consider the problem of minimizing the function $f(x_1, x_2) = x_1 + R^2$ with respect to $x_1$ and $x_2$, subject to the constraint $x_1^2 + x_2^2 \leq R^2$. Obviously, the solution for this problem is $x_1 = -R$, $x_2 = 0$. (a) Write the problem in standard form. (b) Check that the solution satisfies the Kuhn-Tucker conditions at the optimum for $R = 1$. (c) Use the solution at $R = 1$ and the Lagrange multiplier, to predict what the solution will be for $R = 1.5$. Check how accurate is the prediction.

18. Consider the function $f(x) = 3x^4 + 12x^3 + 18x^2 + 12x$. (a) Check that it has a stationary point at $x = -1$. (b) Calculate what kind of stationary point it is. (c) Specify a region where you are sure the function is convex.
19. Consider the problem of minimizing the surface area of a cylinder with a required volume of at least $250\pi$ in$^3$. (a) Formulate the optimization problem in the standard form. (b) Write the optimality conditions (KKT conditions). Use a Lagrange multiplier only for the volume constraint. (c) At the optimum, the height and diameter are both 10 inches. Use this to calculate the Lagrange multiplier. (d) Identify the type of stationary point. (e) Calculate the sensitivity of the optimum surface area to the value of the volume.
20. Consider a function $f(x) = (x - 2)^5$. (a) Check if $f$ has a stationary point at $x = 2$. (b) Classify the definiteness of the Hessian matrix at the stationary point, and classify the stationary point.
21. Consider a function $f(x_1, x_2) = 4 - (x_1 - 2)^2 - (x_2 - 3)^2$. (a) Check if $f$ has a stationary point at $(x_1, x_2) = (2,3)$. (b) Classiful the definiteness of the Hessian matrix at the stationary point, and classify the stationary point.
22. Calculate the derivative of the surface area $f = 2\pi r^2 + 2\pi rh$ with respect to change in volume $g = V = \pi r^2 h$ using the Lagrange multiplier and compare to the derivative obtained by differentiating the exact solution.

23. Consider the problem of maximizing the volume of a cylinder $V = \pi r^2 h$ with a surface area $S = 2\pi r^2 + 2\pi rh$ of no more than $150\pi$ in$^2$. (a) Formulate the optimization problem in the standard form. (b) Write the optimality conditions (KKT conditions). Use a Lagrange multiplier only for the surface constraint. (c) At the optimum, the height and diameter are both 10 inches. Use this to calculate the Lagrange multiplier. (d) Identify the type of stationary point. (e) Calculate the sensitivity of the optimum volume to the value of the surface area constraint.
24. An engineering design problem is formulated as

$$\begin{aligned} &\text{minimize } f(\mathbf{x}) = x_1^2 + 2x_2^2 - 5x_1 - 2x_2 + 10 \\ &\text{subject to } h(\mathbf{x}) = x_1 + 2x_2 - 3 = 0 \\ &\qquad\qquad g(\mathbf{x}) = 3x_1 + 2x_2 - 6 \le 0 \end{aligned}$$

(a) Write KKT necessary condition. (b) How many cases are there to be considered? Identify those cases. (c) Find the solution for the case where $g(\mathbf{x})$ is active. Is this an acceptable case? (d) Suppose the Lagrange multiplier for $h(\mathbf{x}) = 0$ is $\mu = -2$ and that for $g(\mathbf{x}) \le 0$ is $\lambda = 1$. If the constant in $h(\mathbf{x})$ is changed to 3.2 and the constant in $g(\mathbf{x})$ is changed to 6.2, approximate the change of the optimum objective.

25. An engineering design problem is formulated as

$$\begin{aligned} &\text{minimize } f(\mathbf{x}) = px_1 + 4x_2 \\ &\text{subject to } x_1 - 3x_2 \ge -10p \\ &\qquad\qquad x_1 + x_2 \le 6 \\ &\qquad\qquad x_1 - x_2 \le 2 \\ &\qquad\qquad x_1 + 3x_2 \ge 6 \end{aligned}$$

where $x_1$ and $x_2$ non-negative. Use the Kuhn-Tucker conditions to check for (not solve for!) the optimality of the solution $x_1 = 2, x_2 = 4$ for $p = 1$. (Hint: you do not need to worry about inactive constraints in the optimality conditions!). Then, estimate the optimal objective function for $p = 1.1$ without solving the problem again. Estimate how much we can change $p$ before a similarly obtained estimate of the optimum objective function will not work.

26. Classify the stationary points of the following functions: (a) $f(x) = 2x^3 + 3x^2 - 6x + 7$, (b) $f(x) = x$, (c) $f(x) = x^4$, (d) $f(x_1, x_2) = 7 + 2(x_1^3 + x_2^3) - 6x_1x_2$.

27. For the given rational function, determine (a) all stationary points, and (b) check whether the stationary points are strictly local minima using the sufficient conditions

$$f = \frac{x_1 + x_2}{3 + x_1^2 + x_2^2 + x_1x_2}$$

28. A design problem is formulated as

$$\begin{aligned} &\text{minimize } f(\mathbf{x}) = (x_1 - 8)^2 + (x_2 - 5)^2 \\ &\text{subject to } g_1(\mathbf{x}) = 2x_1 - 3x_2 - 4 \le 0 \\ &\qquad\qquad g_2(\mathbf{x}) = 3x_1 + 3x_2 - 16 \le 0 \end{aligned}$$

(a) Construct the Lagrangian and derive the equations for the KKT necessary conditions. (b) How many cases are there to be considered? (c) Consider the cases in which the second inequality constraint $g_2(\mathbf{x})$ is active. Find the point that satisfies the KKT necessary conditions.

29. Consider the following design optimization problem:

$$\begin{aligned} &\text{minimize } f(\mathbf{x}) = x_1^2 + x_2^2 - 4x_1 + 4 \\ &\text{subject to } g_1(x) = -x_1 \le 0 \\ &\qquad\qquad g_2(x) = -x_2 \le 0 \\ &\qquad\qquad g_3(x) = x_2 - (1 - x_1)^3 \le 0 \end{aligned}$$

(a) Find the optimum point graphically. (b) Show that the optimum point does not satisfy the KKT condition. Explain why.

30. Consider the following optimization problem:

$$\begin{aligned} &\text{minimize } f(\mathbf{x}) = (x_1 - 3)^2 + (x_2 - 3)^2 \\ &\text{subject to } g(x) = 2x_1 + x_2 - 2 \le c \\ &\qquad\qquad -x_1 \le 0, -x_2 \le 0 \end{aligned}$$

(a) Find an optimum point and objective function when $c = 0$. (b) Estimate the objective function when $c$ changes to $0.005$, $0.010$, and $0.040$. Compare these estimations with the true optimum objective functions.

31. Answer true or false of the following statements:
    (a) A function can have a negative value at its maximum point.
    (b) If a constant is added to a function, the location of its minimum point can change.
    (c) If the curvature of a function is negative at a stationary point, then the point is a maximum.
32. Find the stationary points of the following functions and classify them: (a) $f(\mathbf{x}) = x_1^2 + 4x_1x_2 + 2x_1x_3 - 7x_2^2 - 6x_2x_3 + 5x_3^2$, (b) $f(\mathbf{x}) = x_1^2 + 2x_2x_3 + x_2^2 + 4x_3^2$, and (c) $f(\mathbf{x}) = 40x_1 + x_1^2x_2 + x_2^2/x_1$.
33. Derive the first-order necessary conditions of a constrained optimization problem with equality constraints using the Lagrange multiplier method.
34. For $f(x, p) = \sin x + px,\ 0 \le x \le 2\pi$, find the minimum for $p = 0$, estimate the derivative $df^*/dp$, and check by solving again for $p = 0.1$ and comparing to finite difference derivative.
35. An optimization problem is to minimize the surface area of a cylinder while the volume of the cylinder must be larger than $128\pi$. Calculate the derivative of the cylinder surface area with respect

to change in volume using the Lagrange multiplier and compare to the derivative obtained by differentiating the exact solution.