
Basic Tools for Reliability Analysis

1.1. Introduction

The modeling of a mechanical system can be defined as the mathematical idealization of physical phenomena that control it. This obviously requires us to define input variables (geometric parameters of the system, loading conditions, etc.) and output variables (displacements, stresses, etc.) that will help to understand the evolution of the mechanical system. The models used are more complex and accurate and the current issue is the identification of the parameters constituting them. In fact, we can no longer afford, in dealing with certain types of problems, to use deterministic models where the mean values interpose only because that generally leads to a very erroneous representation of reality. This chapter presents the basic tools for the development of a model of reliability in biomechanics especially in prosthesis design. This model is considered implicit and requires a numerical simulation to identify the parameters of structural response. To estimate this response, with good accuracy, the finite element method (FEM) appears as a preferential numerical simulation tool. This method consists of discretizing a structure, such as a prosthesis, into a set of subdomains, called finite elements or mesh, linked to each other by nodes. The calculation of a structure is to establish an equation system for the displacements of the set of all meshing nodes and deduct, pursuant to

their resolution, the approximations of the deformation and stress fields. Then, the reliability itself is performed by a process of optimization. To perform the optimization and reliability, a sensitivity analysis is required to determine or identify the role of each parameter with respect to the constraints and objective functions.

1.2. Advantages of numerical simulation and optimization

In general, biomechanical models are very complicated. It is necessary to have tools and methods to design these models for analyzing satisfaction levels. With regard to the mechanical behavior of the structure, the engineer or designer has a wide range of methods: methods based on knowledge (empirical laws, databases, etc.), simplified calculation methods (strength of materials), the FEM which is the most widely used and methods of optimization. The implementation and relevant use of the FEM require a certain experience. However, in a highly competitive industrial context, this method allows us to:

- reduce costs (optimization of shapes and material volumes, choice of materials, reduction of the number of prototypes, etc.);
- reduce the time (reduce the iteration number in the design process, directly propose viable solutions from the behavioral perspective, focus testing, etc.);
- improve the quality (ensure the respect of the various functions and constraints in terms of reliability, comfort, ergonomics, etc.).

The scope of the FEM is very large. They have proved their effectiveness in the case of problems simple such as in that of great complexity calculations. This field covers all applications of the structural mechanics (statics, plasticity, composites, dynamics, shock, friction, etc.) and also the mechanics of fluids, rheology, heat exchange, electromagnetic calculations, etc. [POU 99].

The use of the FEM in the medical field has an additional interest. In fact, contrary to the fields of automotive or aeronautics, the designed products are not intended to equip a car or an airplane but a human being. This induced on the first hand that it is often impossible to test a device on humans as we perform a crash test on a car to test the operation of an airbag, for example. On the second hand, for medical devices, in particular the implantable devices, the reliability is essential because maintenance is not possible. For the design of these devices, the FEM brings not only the advantages mentioned previously (cost, time and quality) but also helps provide the anatomical models (part of the body, biological tissues, etc.). The use of such models is common and can simulate the behavior of devices in location [AOU 10, RAM 11].

1.3. Numerical simulation by finite elements

1.3.1. Use

The design process causes a succession of choices and decisions that lead to the final definition of the product. Numerical simulation has an important role to play in the realization of these choices and can therefore be used at various stages of this process. Depending on the stage of the design, we can differentiate two types of numerical calculation: the calculation for assistance choice and the calculation for validation [POU 99]. The first consists of comparing technical solutions in order to choose the one that meets the criteria set. Contrary to the calculation for validation, it is not the absolute character of the result which is interesting but rather the comparison of the result with that of one or several competing solutions. This type of use allows us to realize simplified models simulations (geometry, behavior laws of materials, etc.). A complete knowledge of the product being not necessary for the simplified model calculation, it may be undertaken in the early stages of the design and prove its interest. In the case of the calculation for validation, the implementation of a numerical simulation requires as a starting point a semi-complete definition of the studied device (forms, dimensions and

materials) and its surroundings (boundary conditions, loads, etc.). It comes at a relatively advanced stage of the project to validate a product definition, and therefore a first set of design choices relative to the specifications. The concept of validation implies a good reliability level of the obtained results. It is therefore appropriate to build a suitable calculation model to reproduce a sufficiently precise mechanical behavior of the piece(s). One step of the model validation is then unavoidable. The use of the FEM for the validation of a product is reflected generally (except some very simple cases) by a fine representation of the geometry and thus a model which is complex and costly in terms of computing resources.

1.3.2. Principle

To treat a problem, FE calculation software requires a certain number of input data. These data consist of a complete description of the mechanical problem to be treated (under a unique formalism to each software) as well as knowledge of the parameters related to the treatment method (for example, the type and distribution of finite elements, the steps of resolution, etc.). The software returns results on the physical quantities of interest in the problem (displacement, temperatures, stresses, etc.). The use of this type of tool therefore requires that the user should be able not only to provide relevant input data, but also to assess the reliability of the obtained results. All that requires a good knowledge of the concerned domain as well as an experience of the theoretical aspects of the method. The problem is considered in the form of a model that first defines the geometry of the structure and the boundary conditions (efforts and displacement). In this case, the FE is more widespread and exploited and it is called the “displacement method”. It consists of determining the “displacement field”, which means the displacement at each point of the structure. In order to represent the displacement field of a structure, the studied field must be discretized using elements of simple geometric shapes (straight line, triangles, quadrangles, tetrahedra, etc.) and of finite dimensions, called “finite elements”. The

set of discretization constitutes the “mesh” of the structure. The displacement approximation is then performed independently on each FE. The accuracy of the results of the calculation is directly related, on the one hand to the choice of elements and on the other hand to the quality of the realized mesh (number of elements, distribution in the structure, shape of elements, etc.).

1.3.3. General approach

In general, the development of a FE model can be described by a succession of steps (Figure 1.1). Some of these steps may differ slightly or be reversed depending on the modeling software used [AOU 11]. The first step is to create the model geometry either by drawing or by importing when there are already files of the STEP, IGES, etc. type. Next, it should be to assign material characteristics to each part of the geometry and then to perform the mesh. The mesh step includes the choice of the element type, their number and distribution depending on the geometry. The next step defines the boundary conditions (loads, displacements, fixations, contacts, etc.). It allows us to recreate utilization conditions of the product or the modeled part. When these four steps are performed, the model is constituted and the calculation can be started. In the case where the calculation is not converged (divergence case), it is necessary to return to the previous steps to refine the different parameters: geometry, behavior laws of materials, mesh, or boundary conditions and loadings.

When the calculation is successful, the numerical results (output data) can be analyzed. Following the development of a FE model, a validation step is essential to prove its credibility. It is therefore essential, as a first step, to simulate a known situation to compare the simulation results with proven results (for example, experimental results) and then to make modifications that will harden the model. Only the correlation of these results allows the validation of the model.

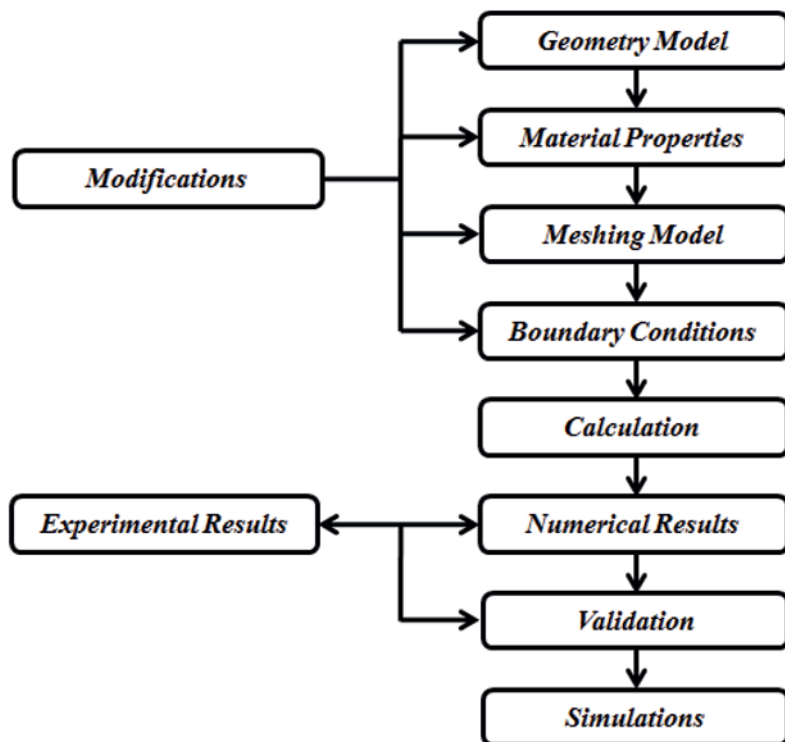


Figure 1.1. General process for developing a finite element model

1.4. Optimization process

The history of optimization is as old as humanity. The first record of optimization being performed was by Heron of Alexandria (Greek engineer, mechanic and mathematician from the first century BC).

“The shortest path that relates a point P to a point Q and that contains a point of a straight line d, is such that at the point of reflection on the straight line d, the incident angle equals to the reflected angle.”

Currently, optimization plays a very important role in operational research and can be applied in several fields (aerospace, automotive and marine industries and recently biomechanics). The constant development of the techniques of computer-aided design and optimization strategies fits within this framework. For example, the optimization of structures for more than 50 years raises the greatest interest. Still too little applied to conventional engineering techniques, it is gradually being introduced and so increasing reliability.

1.4.1. Basic concepts

In mathematics, an optimization problem is to find an element minimizing or maximizing a given function among a given set of data.

1.4.1.1. Optimization parameters

For each optimization problem, we define a set of optimization parameters: objective functions, variables and constraints.

1.4.1.1.1. Objective function

The objective function is a mathematical function of optimization variables. The minimization of this function can be written as follows:

$$\min f(\mathbf{x}) \quad [1.1]$$

It can be a single function ($f(\mathbf{x})$) to minimize, or several functions ($f_1(\mathbf{x}), f_2(\mathbf{x}) \dots$).

1.4.1.1.2. Optimization variables

The optimization variables are a set of variables that govern the situation to be modeled. The vector of variables is given by:

$$\mathbf{x} = \{x_1, x_2, \dots, x_n\} \quad [1.2]$$

The aim is to find the optimal values $\mathbf{x}^* = \{x_1^*, x_2^*, \dots, x_n^*\}$ which minimize the objective function(s).

1.4.1.1.3. Constraints

The constraints define a domain of feasibility. The points that verify constraints belong to the feasibility domain. There are two types of constraints: equality constraints can be written as follows:

$$h_i(\mathbf{x}) = 0 \Leftrightarrow \left\{ \begin{array}{l} h_1(x_1, x_2, \dots, x_n) = 0 \\ h_2(x, x_2, \dots, x_n) = 0 \\ \dots \\ h_j(x, x_2, \dots, x_n) = 0 \end{array} \right\} \quad [1.3]$$

and inequality constraints can be written as follows:

$$g_j(\mathbf{x}) \leq 0 \Leftrightarrow \left\{ \begin{array}{l} g_1(x, x_2, \dots, x_n) \leq 0 \\ g_2(x, x_2, \dots, x_n) \leq 0 \\ \dots \\ g_k(x, x_2, \dots, x_n) \leq 0 \end{array} \right\} \quad [1.4]$$

For example, when mechanical stresses are violated in a structure, there may be a case of failure. In this case, the functions of the mechanical stresses may be considered equality constraints, while the displacement constraints can be considered as constraints of inequality to improve the design.

1.4.1.2. Local or global optimal solutions

A point x^* of the space \mathfrak{R}^n represents a local minimum, if there exists a neighborhood of x^* denoted by $V(x^*)$ such that:

$$\forall x \in V(x^*) \Rightarrow f(x) \geq f(x^*) \quad [1.5]$$

This relation signifies that at the neighborhood of x^* , there exists no point for which $f(x)$ is smaller than $f(x^*)$. A point x^* of the space \mathfrak{R}^n represents a global minimum if:

$$\forall x \in \mathfrak{R}^n \Rightarrow f(x) \geq f(x^*) \quad [1.6]$$

There may be several local optimal solutions, but the global optimal solution is unique and often very difficult to find.

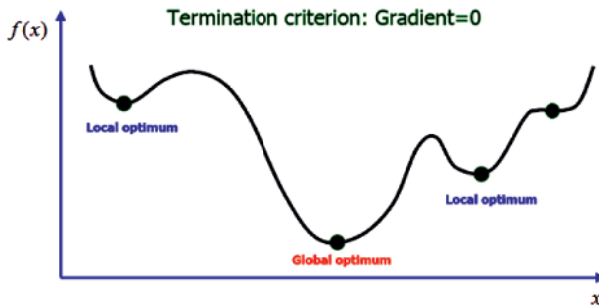


Figure 1.2. Local optimal solutions and a global optimal solution

Figure 1.2 shows several local optimal solutions but there exists only one global optimal solution.

1.4.1.3. Simplified algorithm

The word “algorithm” comes from the name of the Arabic mathematician “Muhammad Ibn Musa AL-KHAWARIZMI” (9th Century), born in Khwarezm in Uzbekistan.

“The algorithm is a finite successive series of rules, to apply in a determined order, to a finite number of data values, in order to arrive with certainty, in a finite number of steps, at a certain result independently of the data”.

The simplified algorithm of the optimization process can be summarized in five stages:

- the first step represents the data input;
- the second step represents the numerical simulation that yields the results;
- the aim of the third step is to compare the results according to the different convergence conditions;

- the fourth step is to improve the objective function by modifying the different optimization variables;
- the final step is to finish the optimization process and show the optimal results.

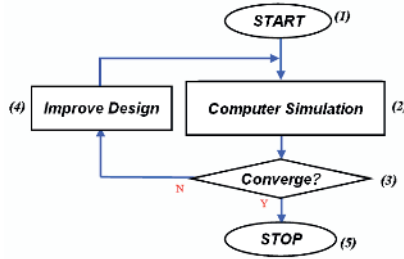


Figure 1.3. Simplified algorithm of the optimization process

Figure 1.3 shows the simplified algorithm of an optimization process and its different stages.

1.4.2. Problem classification

Optimization problems are classified according to several categories: constraint existence, function linearity (objective and constraints) and objective multiplicity.

1.4.2.1. Constraint classification

Optimization problems are classified according to their constraints into two categories: unconstrained and constrained problems.

1.4.2.1.1. Unconstrained problems

Unconstrained optimization has a direct and evident advantage for the identification of peaks (maxima) and troughs (minima), as well as saddle points, before progressing to a more in-depth analysis (peak and trough lines, coarseness, curvatures, geodesics, etc.). The unconstrained optimization problem can be written as follows:

$$\min f(\mathbf{x}) \quad [1.7]$$

The minimization of an objective in the absence of constraints leads to zero values of the components of the first-order derivative vector. If the objective function is nonlinear, a finite solution may exist, even in the absence of constraints. In contrast, the solution is always infinite when the objective function is linear and there are no constraints.

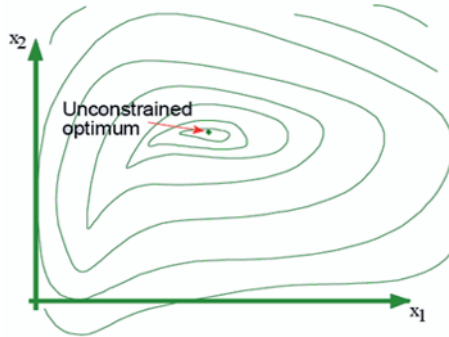


Figure 1.4. Example of an unconstrained optimization problem

Figure 1.4 shows an example of an unconstrained optimization problem, with a global optimum.

1.4.2.1.2. Constrained problems

Although a large number of optimization problems present themselves as constrained optimization problems, they can be reduced to unconstrained problems by an increase of variables (Lagrange multipliers for equality constraints and adjustment variables or gap variable for inequality constraints, as discussed in section 1.4.5.2.1). The optimization problem of an objective under constraints, equalities or inequalities can be written using the following form:

$$\begin{array}{ll}
 \min & :f(\mathbf{x}) \\
 \text{subject to} & :g(\mathbf{x}) \leq 0 \\
 \text{and} & :h(\mathbf{x}) = 0
 \end{array} \quad [1.8]$$

where $h(\mathbf{x})=0$ is the equality constraint and $g(\mathbf{x})\leq 0$ is the inequality constraint.

Figure 1.5 shows an example of a constrained optimization problem with an optimum which can be global.

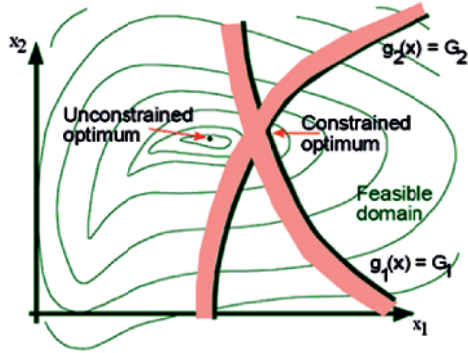


Figure 1.5. Example of a constrained optimization problem

ILLUSTRATIVE EXAMPLE 1.1.—

Consider a cylindrical reservoir (or tank) of diameter D and height H (Figure 1.6). The aim is to minimize the reservoir volume subject to the following conditions:

- the diameter must be between 8 and 3.5 cm;
- the height must be between 18 and 8 cm;
- the minimal volume value must not be below 400 ml.

Write the suitable formulation of this optimization problem.

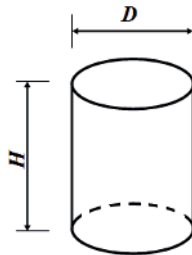


Figure 1.6. Cylindrical reservoir (or tank)

SOLUTION.—

The optimization variables are:

$$x_1 = D, \quad x_2 = H \quad [1.9]$$

The objective as a function of the variables can be written using the following form:

$$f(D, H) = 2 \frac{\pi D^2}{4} + \pi DH, \quad f(x_1, x_2) = \frac{\pi}{2} x_1^2 + \pi \cdot x_1 \cdot x_2 \quad [1.10]$$

The inequality constraints are:

$$g(D, H) = \frac{\pi D^2}{4} H \geq 400 \quad [1.11]$$

$$g(x_1, x_2) = \frac{\pi}{4} x_1^2 \cdot x_2 \geq 400 \quad [1.12]$$

$$g(x_1, x_2) = 1 - \frac{\pi}{1600} x_1^2 \cdot x_2 \leq 0 \quad [1.13]$$

The formulation of this constrained optimization problem is mathematically expressed by:

$$\begin{aligned} \min \quad & f(x_1, x_2) = \frac{\pi}{2} x_1^2 + \pi \cdot x_1 \cdot x_2 \\ \text{subject to} \quad & g(x_1, x_2) = 1 - \frac{\pi}{1600} x_1^2 \cdot x_2 \leq 0 \\ & :3 \leq x_1 \leq 8 \\ & :8 \leq x_2 \leq 18 \end{aligned} \quad [1.14]$$

1.4.2.2. Linearity classification

Optimization problems are classified according to the function linearity (objective and constraints): linear optimization or nonlinear optimization.

1.4.2.2.1. Linear problems

A function $f(x_1, x_2, \dots, x_n)$ of x_1, x_2, \dots, x_n is a linear function if and only if there exists a set of constants c_1, c_2, \dots, c_n such that:

$$f(x_1, x_2, \dots, x_n) = c_1 x_1 + c_2 x_2 \dots + c_n x_n \quad [1.15]$$

In the linear problem, all functions (objective, equality and inequality constraints) must be linear. For example, consider a linear problem expressed by the following form:

$$\begin{aligned} \min : f(x) &= -3x_1 - x_2 \\ \text{s.t.} : \begin{cases} x_2 \leq 9 \\ x_1 = x_2 \end{cases} \end{aligned} \quad [1.16]$$

In this problem, all functions (objective and equality and inequality constraints) are linear (first order).

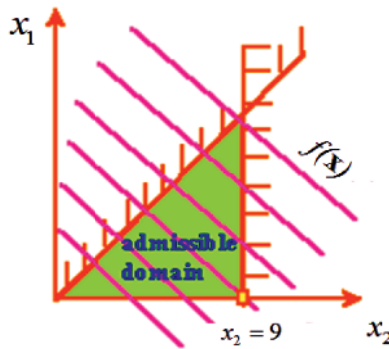


Figure 1.7. Example of a linear problem

Figure 1.7 shows an example of a linear problem where all functions are modeled by straight lines.

1.4.2.2. Nonlinear problems

In a nonlinear problem, one or more functions (objective, equality and inequality constraints) must be nonlinear. For example, consider a nonlinear problem expressed by the following form:

$$\begin{aligned} \min: & f(x) = -3x_1 - x_2 \\ \text{s. t.} : & \begin{cases} x_2 \leq 9 \\ x_1^2 \leq x_2 \end{cases} \end{aligned} \quad [1.17]$$

In this problem, we only have one function that is nonlinear (second order). Although the other functions are linear, we consider this problem to be nonlinear.

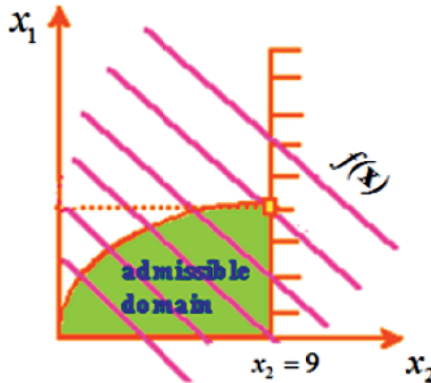


Figure 1.8. Example of a nonlinear problem

Figure 1.8 shows an example of a nonlinear problem where one of the functions is modeled by a second-order curve.

1.4.2.3. Objective classification

Optimization problems can also be classified according to the multiplicity of the objectives: single-objective or multi-objective optimization.

1.4.2.3.1. Single-objective problems

We can easily solve a problem with only one objective and identify the optimal solutions. In this case, the objective is represented by a single component:

$$f(\mathbf{x}) \quad [1.18]$$

Whatever the number of associated constraints, we consider this problem to be single-objective.

1.4.2.3.2. Multi-objective problems

We have several criteria when solving multi-objective problems. In this case, the objective is represented by a vector with multiple components:

$$\begin{Bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ \vdots \\ \vdots \\ f_z(\mathbf{x}) \end{Bmatrix} \quad [1.19]$$

This type of problem is often encountered in biomechanics.

ILLUSTRATIVE EXAMPLE 1.2.—

Consider an optimization problem in the following form:

$$\begin{aligned} & \max_{x,y} 20x + 9y \\ & \text{subject to:} \\ & \quad 3x + y \leq 20 \\ & \quad 2x + y \leq 15 \\ & \quad x, y \geq 0 \end{aligned} \quad [1.20]$$

- classify this optimization problem;
- model geometrically all functions (objective and constraints);
- find the optimal solution.

SOLUTION.—

The classification of this optimization problem is a constrained, linear and single-objective problem.

To model this problem geometrically, we model all functions in the Cartesian space. We start with the function of the first constraint:

$$3x + y \leq 20 \quad [1.21]$$

The intersection of the equation $3x + y = 20$ with the Cartesian axes divides space into two domains: a feasible domain and an infeasible domain (Figure 1.9). To test the two domains, we choose the origin coordinates $(0,0)$.

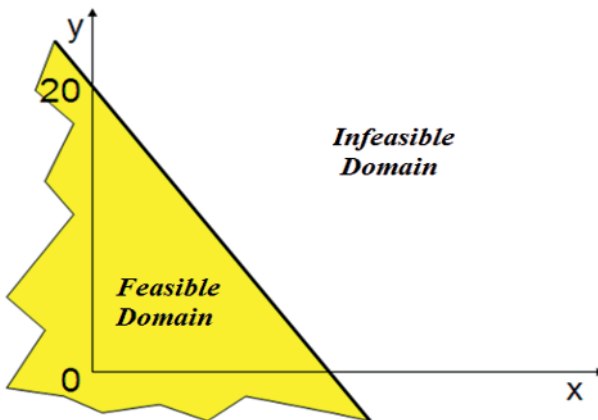


Figure 1.9. Model of the first constraint

Next, we model the function of the second constraint:

$$2x + y \leq 15 \quad [1.22]$$

The intersection of the equation $2x + y = 15$ with the Cartesian axes divides space into two domains: a feasible domain and an infeasible domain.

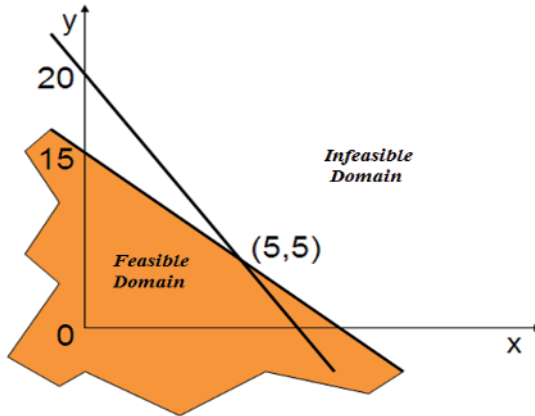


Figure 1.10. Model of the second constraint

Afterward, we find the intersection of the two constraints:

$$\begin{aligned} 3x + y &\leq 20 \\ 2x + y &\leq 15 \end{aligned} \quad [1.23]$$

Figure 1.11 shows the intersection of two straight line segments at the point (5,5).

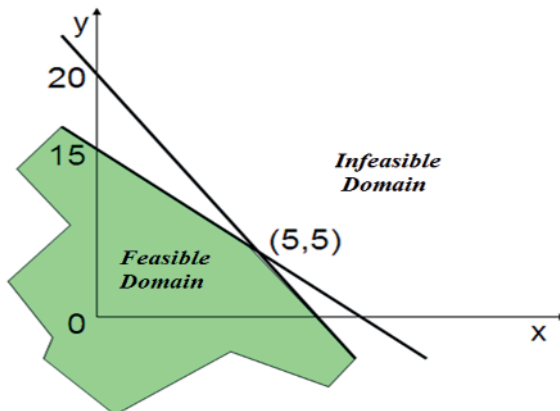


Figure 1.11. Model of the intersection of two constraints

Next, we model all constraints to find the feasible domain:

$$\begin{aligned} 3x + y &\leq 20 \\ 2x + y &\leq 15 \\ x, y &\geq 0 \end{aligned} \quad [1.24]$$

Figure 1.12 shows the intersection of the set of constraints.

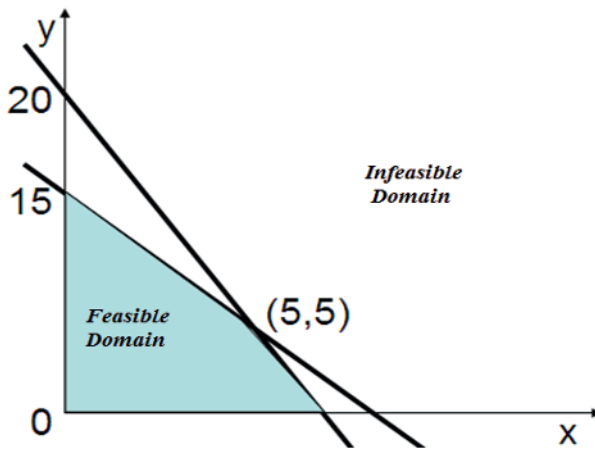


Figure 1.12. Model of the intersection of the set of constraints

Finally, we model the whole problem:

$$\begin{aligned} \max_{x,y} \quad & 20x + 9y \\ \text{subject to:} \quad & \\ & 3x + y \leq 20 \\ & 2x + y \leq 15 \\ & x, y \geq 0 \end{aligned} \quad [1.25]$$

Figure 1.13 shows the model of the iso-values of the objective function ($f(x, y) = 20x + 9y$) with the intersection of the set of constraints.

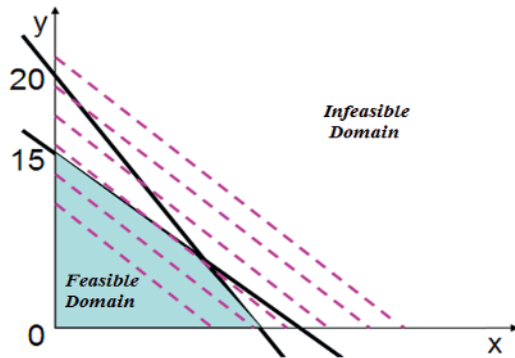


Figure 1.13. Model of the iso-values of the objective function with the set of constraints

Figure 1.14 shows the optimal solution $((x^*, y^*) = (5, 5))$ where the maximal value of the objective is $f(5, 5) = 145$.

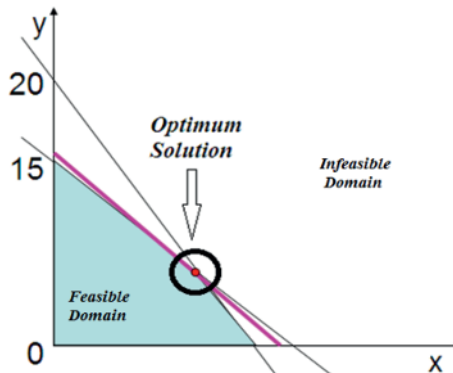


Figure 1.14. Model of the optimal point

ILLUSTRATIVE EXAMPLE 1.3.—

Consider the optimization problem expressed by the following form:

$$\min f(\mathbf{x}) = e^{-x} + x^2 \quad [1.26]$$

- classify this optimization problem;
- model geometrically the objective function $f(\mathbf{x})$;
- find the optimal solution.

SOLUTION.—

The classification of this optimization problem is an unconstrained, nonlinear, single-objective problem.

To model this function geometrically, we calculate the function for several values of the variable x (Table 1.1).

x	0	0.5	1	2	3
$f(x)$	1	0.83	1.36	4.13	9.03

Table 1.1. *Objective function evaluation for different variable values*

We observe that the objective function changes its direction when considering the different values of the variable x . In order to determine the minimum value of the objective function, we can analytically calculate its derivative as follows:

$$\frac{\partial f}{\partial x} = -e^{-x} + 2x \quad [1.27]$$

Considering the null value of the derivative, we obtain:

$$x = \frac{1}{2}e^{-x} \quad [1.28]$$

This equation can be solved using iterative techniques (Table 1.2).

Iteration	0	1	2	3	4	5	6	7	8
x	0	0.5	0.303	0.369	0.349	0.354	0.350	0.351	0.351

Table 1.2. *Iterative values until convergence*

The optimal value of the function is $f(x^*)=0.828$ when $x^{(8)}=0.351$. Figure 1.15 shows the geometrical interpretation of the objective function and the optimal value of the variable x .

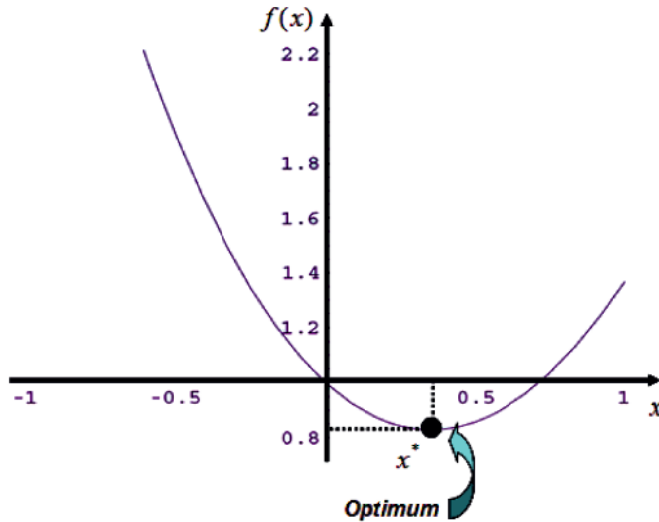


Figure 1.15. Objective function interpretation and the optimum value

1.4.3. Optimization methods

We select an optimization method according to the following four criteria:

- the *generality* is the potential to use the method in different applications;
- the *robustness* is the capacity of the method to find optimal solutions regardless of the starting points;
- the *efficiency* is the speed of the method to find optimal solutions;
- the *capacity* is the potential to deal with a large number of variables and constraints.

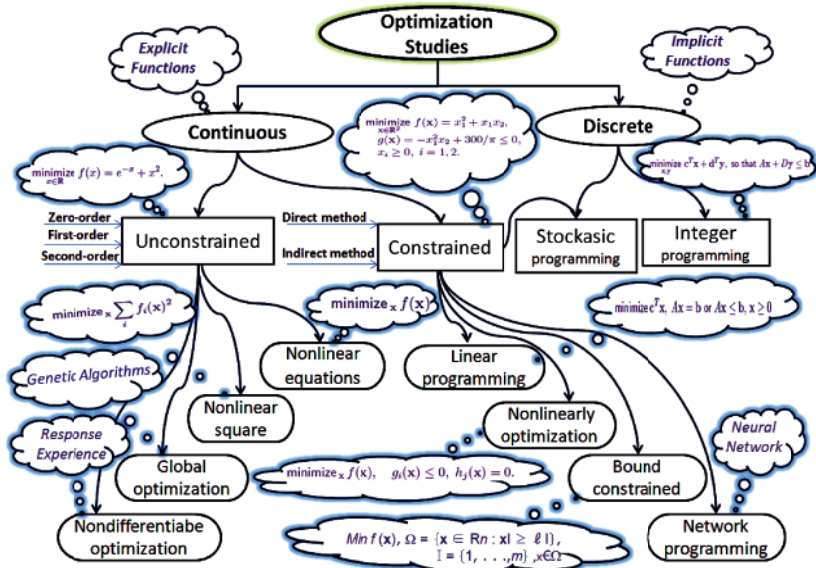


Figure 1.16. Optimization strategies

Figure 1.16 presents the different aspects of the optimization process to be studied. In general, we divide the optimization studied into two categories: continuous and discrete optimization [KHA 11]. The continuous optimization needs several analytical competences to simplify the studied problem before solving it, while the discrete optimization necessitates a good computing technology to solve the studied problem.

1.4.4. Unconstrained methods

The majority of optimization problems are solved by this type of method. This is partly because constrained optimization problems can be reduced to unconstrained problems. The main advantage of these methods is their potential to be implemented on a machine by a single loop. In this chapter, we only present three categories of these methods.

1.4.4.1. Zero-order methods

In this type of method, we use iterative evaluations of functions. We never use the derivatives of functions. These methods can be used for discontinuous and/or non-differentiable functions.

1.4.4.1.1. Simplex method

This method is principally used to solve linear problems. The idea is to calculate three points and then find the direction of the optimal solution as is shown in Figure 1.17.

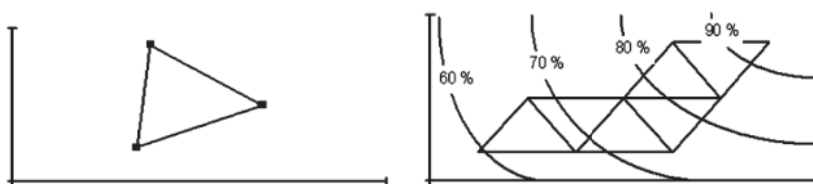


Figure 1.17. Principle of the simplex method

1.4.4.1.2. Curve fitting method

The principle of this method is based upon curve approximation techniques, which are different relative to the interpolation techniques. The main difference is that the resulting smooth curves should not pass through the used experiment points.

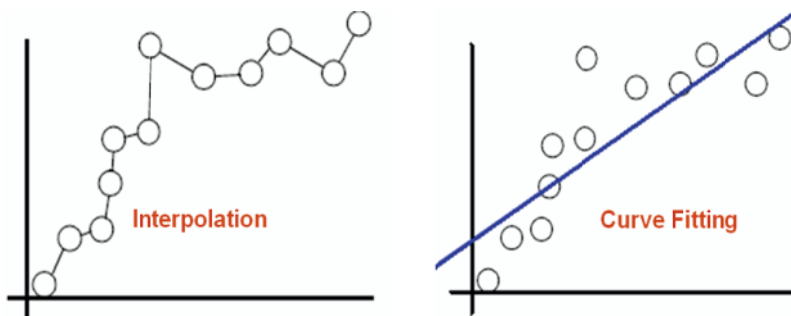


Figure 1.18. Interpolation and the curve fitting approximation

Figure 1.18 shows the difference between the approximation and interpolation methods.

1.4.4.2. First-order methods

The principle of this type of method is to use the first-order derivative and a progress (forward) step to arrive to the optimal solution. The main algorithm consists of:

- initializing the start point: $k = 0$ and \mathbf{x}_0 ;
- solving for the research direction: \mathbf{s}_0 ;
- evaluating the subsequent point using the equation:
 $\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_{k+1} \mathbf{s}_k$;
- passing to the following iteration: $k = k + 1$;
- while $|x_k - x_{k-1}| > \varepsilon$.

1.4.4.2.1. Descent gradient method

The descent gradient method (DGM) is based upon the first-order derivative and a progress step. The principal equation is expressed by the following:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - a_{k+1} \mathbf{s}_k \quad [1.29]$$

with the iteration $k = 0, 1, 2, \dots, n$ and the search direction is expressed using the following form:

$$\mathbf{d}_{k+1} = \mathbf{x}_{k+1} - \mathbf{x}_k = -a_{k+1} \mathbf{s}_k \quad [1.30]$$

Here, the search direction is evaluated using the first-order derivative as follows:

$$\mathbf{s}_k = \nabla \mathbf{f}(\mathbf{x}_k) \quad [1.31]$$

and the step size can be calculated by:

$$a_{k+1} = \frac{df(a_{k+1})}{d a_{k+1}}, \quad k = 0, 1, 2, \dots, n \quad [1.32]$$

This method has a slow progress and requires a significant computation time.

1.4.4.2.2. Conjugate gradient method

The principle of the conjugate gradient method (CGM) is based upon the evaluation of the first order for the first step ($k = 0$):

$$\mathbf{s}_k = \nabla \mathbf{f}(\mathbf{x}_k) \quad [1.33]$$

However, use:

$$\mathbf{s}_{k+1} = \nabla \mathbf{f}(\mathbf{x}_{k+1}) + \beta_{k+1} \mathbf{s}_k \quad [1.34]$$

where the coefficient β can be calculated by:

$$\beta = \frac{\langle \nabla \mathbf{f}(\mathbf{x}_{k+1}) \rangle \{ \nabla \mathbf{f}(\mathbf{x}_{k+1}) \}}{\langle \nabla \mathbf{f}(\mathbf{x}_k) \rangle \{ \nabla \mathbf{f}(\mathbf{x}_k) \}} = \frac{\| \nabla \mathbf{f}(\mathbf{x}_{k+1}) \|^2}{\| \nabla \mathbf{f}(\mathbf{x}_k) \|^2} \quad [1.35]$$

In this case, we can use two derivatives in two successive steps. Figure 1.19 shows a geometric interpretation of an example of two variables when considering the DGM and CGM.

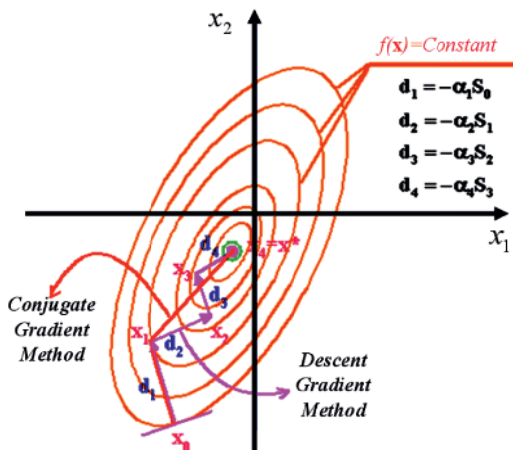


Figure 1.19. Comparison of the descent gradient and conjugated gradient methods

For the same starting point \mathbf{x}_0 , the DGM requires four iterations to arrive at the optimal point \mathbf{x}^* , while the CGM only needs two iterations.

1.4.4.3. Second-order methods

This type of method requires the evaluation of second-order derivatives. We use a matrix known as the Hessian Matrix as follows:

$$\mathbf{H}(\mathbf{x}_0) = \nabla^2 \mathbf{f}(\mathbf{x}_0) = \left\{ \begin{array}{cccc} \frac{\partial^2 f}{\partial x_1^2}(\mathbf{x}_0) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(\mathbf{x}_0) & \dots & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n}(\mathbf{x}_0) \\ \frac{\partial^2 f}{\partial x_1 \partial x_2}(\mathbf{x}_0) & \ddots & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n}(\mathbf{x}_0) & \dots & \dots & \dots & \frac{\partial^2 f}{\partial x_n^2}(\mathbf{x}_0) \end{array} \right\} \quad [1.36]$$

Despite this type of method having a good level of efficiency, it is considered very sensitive and can lead to instabilities.

1.4.4.3.1. Newton's method

Isaac Newton (1643–1727) was an English physicist, astronomer and mathematician. He is often considered to be the most influential scientist of all time. His contributions include differential calculus, algebra, analytic geometry, his law of gravitation and laws of planetary motion.

Newton's method (NM) is also based upon the basic iterative equation as follows:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - a_{k+1} \mathbf{s}_k \quad [1.37]$$

However, the search direction depends on the Hessian matrix as follows:

$$\{\mathbf{s}_k\} = [H(\mathbf{x}_k)]^{-1} \{\nabla f(\mathbf{x}_k)\} \quad [1.38]$$

We consider the following forward step:

$$a_{k+1} = 1 \quad [1.39]$$

Hence, the iterative equation can be written as follows:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - [H(\mathbf{x}_k)]^{-1} \{\nabla f(\mathbf{x}_k)\} \quad [1.40]$$

NM is efficient but suffers from a repeated calculation of the Hessian matrix at each iteration.

1.4.4.3.2. Modified Newton's method

The modified Newton's method (MNM) requires a single calculation of the Hessian matrix at the first iteration. The iterative equation is written using the following form:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_{k+1} [H(\mathbf{x}_0)]^{-1} \{\nabla f(\mathbf{x}_k)\} \quad [1.41]$$

with a search direction:

$$\mathbf{s}_k = [H(\mathbf{x}_0)]^{-1} \{\nabla f(\mathbf{x}_k)\} \quad [1.42]$$

If $\mathbf{s}_k = \{\nabla f(\mathbf{x}_k)\}$, we return to the DGM, and if $\alpha_{k+1} = 1$ and $\mathbf{s}_k = [H(\mathbf{x}_k)]^{-1} \{\nabla f(\mathbf{x}_k)\}$, we return to NM.

ILLUSTRATIVE EXAMPLE 1.4.–

Consider an unconstrained optimization problem using the following form:

$$\min : f(\mathbf{x}) = x_1 - x_2 + 2x_1^2 + 2x_1x_2 + x_2^2 \quad [1.43]$$

– find the minimal value using first- and second-order methods using the starting point $\mathbf{x}_0 = (0, 0)$;

– compare the different methods according to computing time.

SOLUTION.–

We start with the first-order methods (DGM and CGM), then the second-order methods (NM and MNM).

Descent gradient method

We first find the first-order derivative of the objective function $f(\mathbf{x})$:

$$\nabla f(\mathbf{x}) = \begin{Bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \end{Bmatrix} = \begin{Bmatrix} 1 + 4x_1 + 2x_2 \\ -1 + 2x_1 + 2x_2 \end{Bmatrix} \quad [1.44]$$

Next, we calculate the search direction for the initial point:

$$S_0 = \nabla f(\mathbf{x}_0) = \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} \quad [1.45]$$

By substituting this result into the iterative equation, we obtain:

$$x_{(1)} = x_{(0)} - \alpha_1 S_0 \quad [1.46]$$

When considering the forward step as a variable, we obtain:

$$x_{(1)} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} - \alpha_1 \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} = \begin{Bmatrix} -\alpha_1 \\ \alpha_1 \end{Bmatrix} \quad [1.47]$$

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha_1) = -\alpha_1 - \alpha_1 + 2\alpha_1^2 - 2\alpha_1^2 + \alpha_1^2 = +\alpha_1^2 - 2\alpha_1 \quad [1.48]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha_1)}{\partial \alpha_1} = 2\alpha_1 - 2 = 0 \Rightarrow \alpha_1 = 1 \quad [1.49]$$

The new value is:

$$x_{(1)} = \begin{Bmatrix} -1 \\ 1 \end{Bmatrix} \quad [1.50]$$

Figure 1.20 shows the coordinates of the new value at iteration (1).

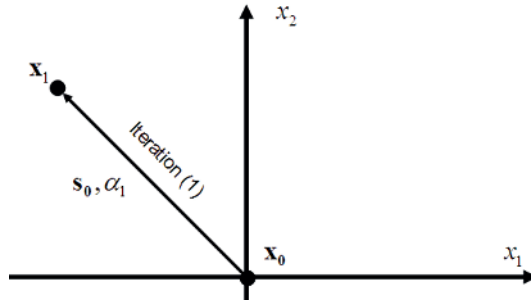


Figure 1.20. Iteration (1) using DGM

Next, we calculate the search direction for iteration 1:

$$S_1 = \nabla f(\mathbf{x}_1) = \begin{Bmatrix} -1 \\ -1 \end{Bmatrix} \quad [1.51]$$

By substituting this result into the iterative equation, we obtain:

$$x_{(2)} = x_{(1)} - \alpha_2 S_{(1)} \quad [1.52]$$

When considering the forward step as a variable, we obtain:

$$x_{(2)} = \begin{Bmatrix} -1 \\ 1 \end{Bmatrix} - \alpha_2 \begin{Bmatrix} -1 \\ -1 \end{Bmatrix} = \begin{Bmatrix} -1 + \alpha_2 \\ +1 + \alpha_2 \end{Bmatrix} \quad [1.53]$$

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha_2) = (-1 + \alpha_2) - (1 + \alpha_2) + 2(-1 + \alpha_2)^2 + 2(-1 + \alpha_2)(1 + \alpha_2) + (1 + \alpha_2)^2 \quad [1.54]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha_2)}{\partial \alpha_2} = -10\alpha_2 - 2 = 0 \Rightarrow \alpha_2 = \frac{1}{5} \quad [1.55]$$

The new value is:

$$x_{(2)} = \begin{Bmatrix} -0.8 \\ 1.2 \end{Bmatrix} \quad [1.56]$$

Figure 1.21 shows the coordinates of the new value at iteration (2).

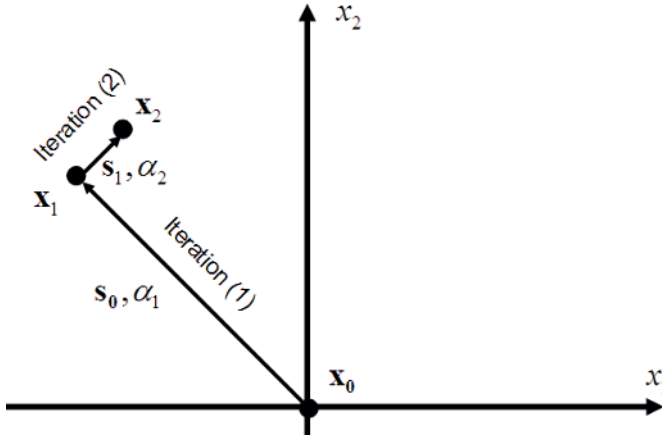


Figure 1.21. Iteration (2) using DGM

Next, we calculate the search direction for iteration 2:

$$S_{(2)} = \nabla f(x_2) = \begin{Bmatrix} 0.2 \\ -0.2 \end{Bmatrix} \quad [1.57]$$

By substituting this result into the iterative equation, we obtain:

$$x_{(3)} = x_{(2)} - \alpha_3 S_{(2)} \quad [1.58]$$

When considering the forward step as a variable, we obtain:

$$x_{(3)} = \begin{Bmatrix} -0.8 \\ 1.2 \end{Bmatrix} - \alpha_3 \begin{Bmatrix} 0.2 \\ -0.2 \end{Bmatrix} = \begin{Bmatrix} -0.8 - 0.2\alpha_3 \\ 1.2 + 0.2\alpha_3 \end{Bmatrix} \quad [1.59]$$

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha_3) = (-0.8 - 0.2\alpha_3) - (1.2 + 0.2\alpha_3) + 2(-0.8 - 0.2\alpha_3)^2 + 2(-0.8 - 0.2\alpha_3)(1.2 + 0.2\alpha_3) + 2(1.2 + 0.2\alpha_3)^2 \quad [1.60]$$

The obtained equation can be simplified into the following form:

$$f(\alpha_3) = 0.24 + 0.4\alpha_3 + 0.08\alpha_3^2 \quad [1.61]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha_3)}{\partial \alpha_3} = 0.4 + 0.16\alpha_3 = 0 \Rightarrow \alpha_3 = -2.5 \quad [1.62]$$

The new value is:

$$\mathbf{x}_{(3)} = \begin{Bmatrix} -0.3 \\ 0.7 \end{Bmatrix} \quad [1.63]$$

Figure 1.22 shows the coordinates of the new value at iteration (3).

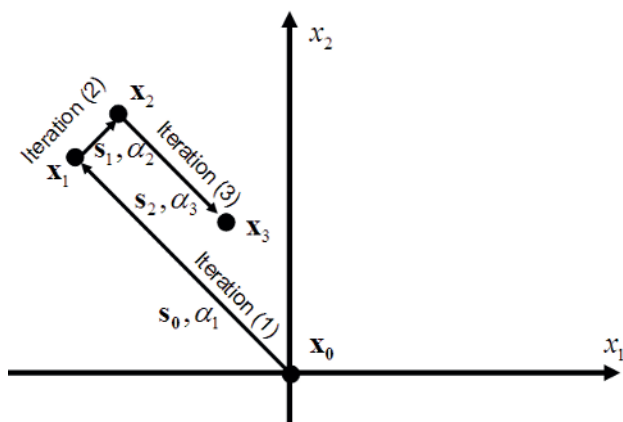


Figure 1.22. Iteration (3) using DGM

Next, we calculate the search direction for iteration 3:

$$S_{(3)} = \nabla f(\mathbf{x}_3) = \begin{Bmatrix} 1.2 \\ -0.2 \end{Bmatrix} \quad [1.64]$$

By substituting this result into the iterative equation, we obtain:

$$\mathbf{x}_{(4)} = \mathbf{x}_{(3)} - \alpha_4 S_{(3)} \quad [1.65]$$

When considering the forward step as a variable, we obtain:

$$\mathbf{x}_{(4)} = \begin{Bmatrix} -0.3 \\ 0.7 \end{Bmatrix} - \alpha_4 \begin{Bmatrix} 1.2 \\ -0.2 \end{Bmatrix} = \begin{Bmatrix} -0.3 - 1.2\alpha_4 \\ 0.7 + 0.2\alpha_4 \end{Bmatrix} \quad [1.66]$$

Figure 1.23 shows the coordinates of the new value at iteration (4).

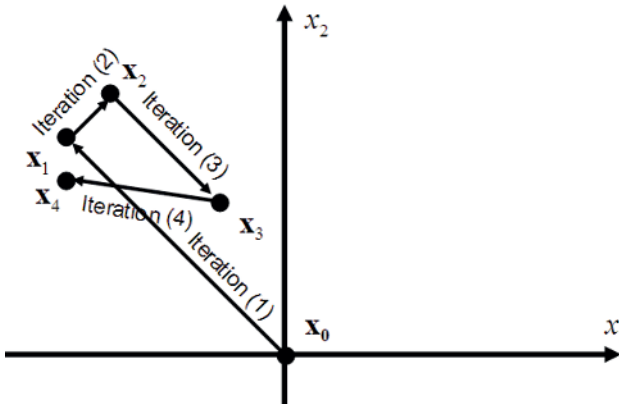


Figure 1.23. Iteration (4) using DGM

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha_4) = (-0.3 - 1.2\alpha_4) - (0.7 + 0.2\alpha_4) + 2(-0.3 - 1.2\alpha_4)^2 + 2(-0.3 - 1.2\alpha_4)(0.7 + 0.2\alpha_4) + 2(0.7 + 0.2\alpha_4)^2 \quad [1.67]$$

The obtained equation can be simplified into the following form:

$$f(\alpha_4) = 1.04\alpha_4^2 - 1.2\alpha_4 - 0.26 \quad [1.68]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha_4)}{\partial \alpha_4} = 2.08\alpha_4 - 1.2 = 0 \Rightarrow \alpha_4 = 0.58 \quad [1.69]$$

The new value is:

$$\mathbf{x}_{(4)} = \begin{Bmatrix} -0.996 \\ 0.816 \end{Bmatrix} \quad [1.70]$$

Next, we calculate the search direction for iteration 4:

$$S_{(4)} = \nabla f(\mathbf{x}_4) = \begin{Bmatrix} -1.352 \\ -1.36 \end{Bmatrix} \quad [1.71]$$

By substituting this result into the iterative equation, we obtain:

$$x_{(5)} = x_{(4)} - \alpha_5 S_4 \quad [1.72]$$

When considering the forward step as a variable, we obtain:

$$x_{(5)} = \begin{Bmatrix} -0.996 \\ 0.816 \end{Bmatrix} - \alpha_5 \begin{Bmatrix} -1.352 \\ -1.36 \end{Bmatrix} = \begin{Bmatrix} -0.996 + 1.352\alpha_5 \\ 0.816 + 1.36\alpha_5 \end{Bmatrix} \quad [1.73]$$

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha_5) = (-0.996 + 1.352\alpha_5) - (0.816 + 1.36\alpha_5) + 2(-0.996 + 1.352\alpha_5)^2 + 2(-0.996 + 1.352\alpha_5)(0.816 + 1.36\alpha_5) + 2(0.816 + 1.36\alpha_5)^2 \quad [1.74]$$

The equation obtained can be simplified into the following form:

$$f(\alpha_5) = -0.122 - 3.078\alpha_5 + 11.02\alpha_5^2 \quad [1.75]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha_5)}{\partial \alpha_5} = 22.04\alpha_5 - 3.078 = 0 \Rightarrow \alpha_5 = 0.14 \quad [1.76]$$

The new value is:

$$\mathbf{x}_{(5)} = \begin{Bmatrix} -0.8 \\ 1 \end{Bmatrix} \quad [1.77]$$

Figure 1.24 shows the coordinates of the new value at iteration (5).

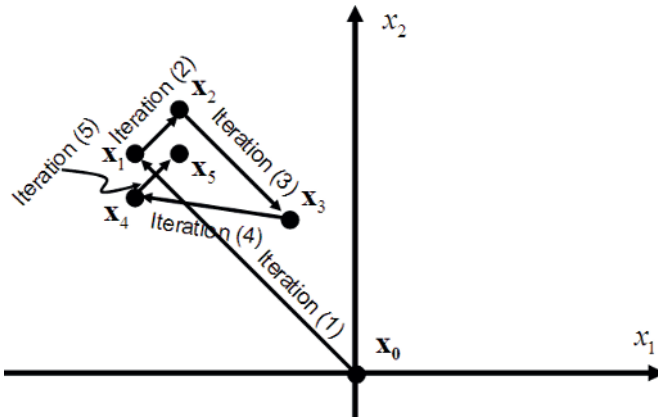


Figure 1.24. Iteration (5) using DGM

Next, we calculate the search direction for iteration 5:

$$S_{(5)} = \nabla f(\mathbf{x}_5) = \begin{Bmatrix} -0.2 \\ -0.6 \end{Bmatrix} \quad [1.78]$$

By substituting this result into the iterative equation, we obtain:

$$x_{(6)} = x_{(5)} - \alpha_6 S_5 \quad [1.79]$$

When considering the forward step as a variable, we obtain:

$$x_{(6)} = \begin{Bmatrix} -0.8 \\ 1 \end{Bmatrix} - \alpha_6 \begin{Bmatrix} -0.2 \\ -0.6 \end{Bmatrix} = \begin{Bmatrix} -0.8 + 0.2\alpha_6 \\ 1 + 0.6\alpha_6 \end{Bmatrix} \quad [1.80]$$

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha_6) = (-0.8 + 0.2\alpha_6) - (1 + 0.6\alpha_6) + 2(-0.8 + 0.2\alpha_6)^2 + 2(-0.8 + 0.2\alpha_6)(1 + 0.6\alpha_6) + (1 + 0.6\alpha_6)^2 \quad [1.81]$$

The obtained equation can be simplified into the following form:

$$f(\alpha_6) = 1.04\alpha_6^2 + 0.8\alpha_6 - 0.12 \quad [1.82]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha_6)}{\partial \alpha_6} = 1.04\alpha_6 + 0.8 = 0 \Rightarrow \alpha_6 = 0.77 \quad [1.83]$$

The new value is:

$$\mathbf{x}_{(6)} = \begin{Bmatrix} -1 \\ 1.5 \end{Bmatrix} \quad [1.84]$$

At the optimal point, we find that the derivative is null:

$$\nabla f(\mathbf{x}_6) = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \quad [1.85]$$

Figure 1.25 shows the coordinates of the new value at iteration (6).

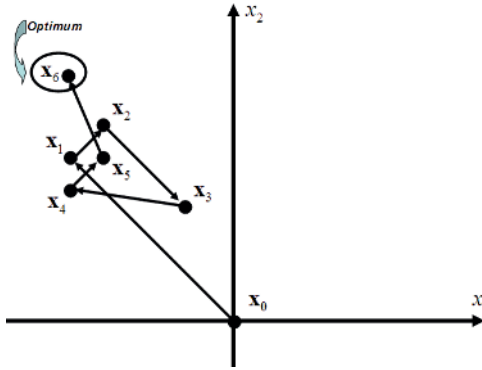


Figure 1.25. Iteration (6) using DGM

Conjugate gradient method

We calculate the search direction for the initial point considering the derivative as follows:

$$S_0 = \nabla f(\mathbf{x}_0) = \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} \quad [1.86]$$

When considering the forward step as a variable, we obtain:

$$x_{(1)} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} - \alpha_1 \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} = \begin{Bmatrix} -\alpha_1 \\ \alpha_1 \end{Bmatrix} \quad [1.87]$$

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha_1) = -\alpha_1 - \alpha_1 + 2\alpha_1^2 - 2\alpha_1^2 + \alpha_1^2 = +\alpha_1^2 - 2\alpha_1 \quad [1.88]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha_1)}{\partial \alpha_1} = 2\alpha_1 - 2 = 0 \Rightarrow \alpha_1 = 1 \quad [1.89]$$

The new value is:

$$x_{(1)} = \begin{Bmatrix} -1 \\ 1 \end{Bmatrix} \quad [1.90]$$

The second stage deals with calculating the coefficient β . Here, we determine the derivative at this point:

$$S_1 = \nabla f(\mathbf{x}_1) = \begin{Bmatrix} -1 \\ -1 \end{Bmatrix} \quad [1.91]$$

Next, we calculate the coefficient β using the following equation:

$$\beta_{k+1} = \frac{\langle \nabla f(x_k) \rangle \{ \nabla f(x_k) \}}{\langle \nabla f(x_{k-1}) \rangle \{ \nabla f(x_{k-1}) \}} = \frac{\langle -1 \quad -1 \rangle \begin{Bmatrix} -1 \\ -1 \end{Bmatrix}}{\langle 1 \quad -1 \rangle \begin{Bmatrix} 1 \\ -1 \end{Bmatrix}} = 1 \quad [1.92]$$

The search direction can then be written as follows:

$$\{S\}_{k+1} = \nabla \{f(x)\}_{k+1} + \beta_{k+1} \{S\}_k \quad [1.93]$$

The search direction for this iteration is:

$$S_1 = \begin{Bmatrix} -1 \\ -1 \end{Bmatrix} + 1 \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} = \begin{Bmatrix} 0 \\ -2 \end{Bmatrix} \quad [1.94]$$

The iterative equation becomes:

$$x_{(2)} = x_{(1)} - \alpha_2 S_1 \quad [1.95]$$

When considering the forward step as a variable, we obtain:

$$x_{(2)} = \begin{Bmatrix} -1 \\ 1 \end{Bmatrix} - \alpha_2 \begin{Bmatrix} 0 \\ -2 \end{Bmatrix} = \begin{Bmatrix} -1 \\ 1 + 2\alpha_2 \end{Bmatrix} \quad [1.96]$$

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha_2) = -1 - (1 + 2\alpha_2) + 2(-1)^2 + 2(-1)(1 + 2\alpha_2) + (1 + 2\alpha_2)^2 \quad [1.97]$$

The equation obtained can be simplified into the following form:

$$f(\alpha_2) = -1 - 2\alpha_2 + 4\alpha_2^2 \quad [1.98]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha_2)}{\partial \alpha_2} = -2 + 8\alpha_2 = 0 \Rightarrow \alpha_2 = \frac{1}{4} \quad [1.99]$$

The new value is:

$$\mathbf{x}_{(2)} = \begin{Bmatrix} -1 \\ 1.5 \end{Bmatrix} \quad [1.100]$$

At the optimal point, we find that the derivative is null:

$$\nabla f(\mathbf{x}_{(2)}) = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \quad [1.101]$$

Figure 1.26 shows the coordinates of the new value at iteration (2).

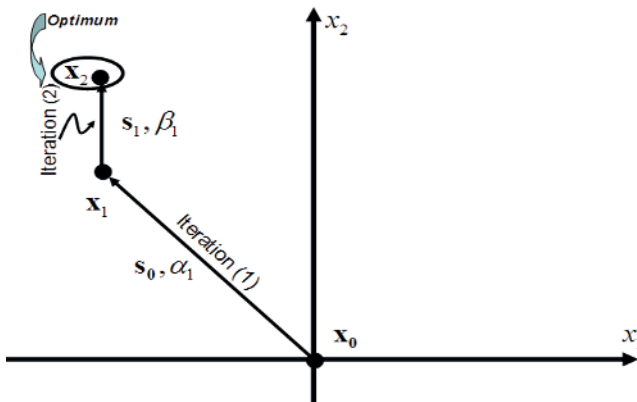


Figure 1.26. Iterations 1 and 2 using CGM

Newton's method

The second-order methods are generally efficient to find the optimal solutions. They use calculations of second-order gradients. We calculate the first-order derivative:

$$S_0 = \nabla f(\mathbf{x}_0) = \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} \quad [1.102]$$

Then, we calculate the Hessian matrix as follows:

$$H(x_0) = \begin{bmatrix} \frac{\partial^2 f(x_0)}{\partial x_1^2} & \frac{\partial^2 f(x_0)}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f(x_0)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x_0)}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix} \quad [1.103]$$

Next, the inverse of this matrix (see Appendix 1) is then:

$$H(x_0)^{-1} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{bmatrix} \quad [1.104]$$

Hence, the search direction can be expressed by:

$$d_{k+1} = x_{k+1} - x_k = -[H(x_k)]^{-1} \nabla f(x_k) \quad [1.105]$$

and the iterative equation is expressed as:

$$x_1 = x_0 - [H(x_0)]^{-1} \nabla f(x_0) \quad [1.106]$$

Considering the iterative equation, we obtain:

$$x_1 = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} - \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{bmatrix} \begin{Bmatrix} 1 \\ -1 \end{Bmatrix}^* \quad [1.107]$$

The new value is thus:

$$x_1 = \begin{Bmatrix} -1 \\ 3 \\ 2 \end{Bmatrix} \quad [1.108]$$

At the optimal point, we find that the derivative is null:

$$\nabla f(\mathbf{x}_1) = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \quad [1.109]$$

NM converges after a single iteration.

Modified Newton's method

This method only uses the Hessian matrix for the first iteration. We obtain the inverse of the Hessian matrix as before (see equation [1.104]). However, we introduce the step to the iterative equation as follows:

$$x_{(1)} = x_{(0)} - \alpha [H(x_0)]^{-1} \nabla f(x_0) \quad [1.110]$$

When considering the forward step as a variable, we obtain:

$$x_{(1)} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} - \alpha \begin{bmatrix} 0.5 & -0.5 \\ -0.5 & 1 \end{bmatrix} \begin{Bmatrix} 1 \\ -1 \end{Bmatrix} = \begin{Bmatrix} -\alpha \\ 1.5\alpha \end{Bmatrix} \quad [1.111]$$

We calculate the forward step by substituting the optimization variables in the objective function formulation as follows:

$$f(\alpha) = -\alpha - 1.5\alpha + 2(-\alpha)^2 + 2(-\alpha)(1.5\alpha) + (1.5)^2 \alpha^2 \quad [1.112]$$

The obtained equation can be simplified into the following form:

$$f(\alpha) = -2.5\alpha + 1.25\alpha^2 \quad [1.113]$$

The derivative of the iterative equation with respect to the current step gives:

$$\frac{\partial f(\alpha)}{\partial \alpha} = 2.5\alpha - 2.5 = 0 \Rightarrow \alpha = 1 \quad [1.114]$$

The new value is:

$$\mathbf{x}_{(1)} = \begin{Bmatrix} -1 \\ 1.5 \end{Bmatrix} \quad [1.115]$$

At the optimal point, we find that the derivative is null:

$$\nabla f(\mathbf{x}_1) = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \quad [1.116]$$

Figure 1.27 shows the coordinates of the new value at iteration (1).

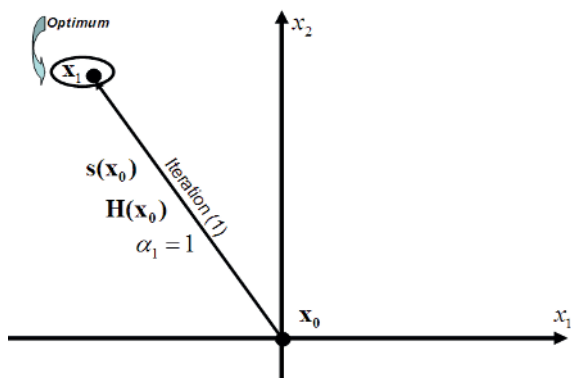


Figure 1.27. Iteration (1) using NM and MNM

The initial value of the objective is $f(\mathbf{x}_0) = 0$, while the minimal value is $f(\mathbf{x}^*) = -0.5$.

This equation can be solved using iterative techniques.

Method	DGM	CGM	NM	MNM
Iterations	6	2	1	1

Table 1.3. Number of iterations for the different methods

Table 1.3 shows a comparison between the four methods used. For this example, the CGM is very efficient relative to the DGM. Although the second-order methods only require one iteration, the evaluation of the Hessian matrix is a potential issue during optimization.

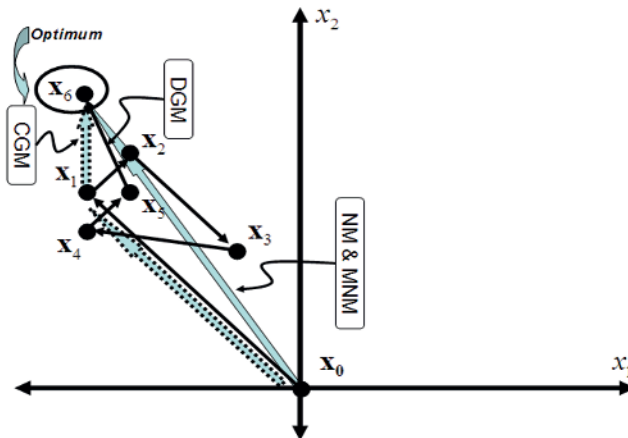


Figure 1.28. Different iterations for the different methods

Figure 1.28 shows the different iterations (trajectories) for the different methods used.

1.4.5. Constrained methods

In general, constrained optimization methods can be divided into two categories: direct methods and transformation methods.

1.4.5.1. Direct methods

The direct methods use linear or nonlinear programming techniques.

1.4.5.1.1. SLP method

The sequential linear programming or successive linear programming (SLP) is an optimization technique for approximately

solving nonlinear optimization problems method. When starting at some estimate of the optimal solution, the method is based on solving a sequence of first-order approximations (i.e. linearizations) of the model. The linearizations are linear programming problems, which can be solved efficiently.

1.4.5.1.2. SQP method

SQP methods solve a sequence of optimization subproblems, each of which optimizes a quadratic model of the objective function subject to a linearization of the constraints. If the problem is unconstrained, then the method reduces to NM for finding a point where the gradient of the objective vanishes. If the problem has only equality constraints, then the method is equivalent to applying NM to the first-order optimality conditions of the problem. SQP methods have been implemented in many packages such as MATLAB.

1.4.5.2. Transformation methods

These methods transform constrained problems into new formulations by increasing the number of variables.

1.4.5.2.1. Lagrange method

Joseph-Louis Comte de Lagrange (1736–1813) was a French mathematician, born in Italy. He worked on isoparametric problems, founded calculus of variations and contributed to calculus of probabilities, the theory of equations and group theory.

The Lagrange method uses Lagrange multipliers for equality constraints, and adjustment variables or slack variables for inequality constraints. The Lagrange formulation of a constrained optimization problem can be written using the following form:

$$L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\mathbf{x}) + \sum_{j=1}^L \lambda_j h_j(\mathbf{x}) + \sum_{k=1}^m \mu_k g_k(\mathbf{x}) \quad [1.117]$$

The Lagrange formulation is a function of \mathbf{x} , λ and μ . To solve this problem, we use unconstrained methods.

ILLUSTRATIVE EXAMPLE 1.5.–

Consider an optimization problem of the following form:

$$\begin{aligned} \min f(\mathbf{x}) &= -3x_1 - x_2, \\ \text{subject to } &\begin{cases} -6x_1 + 5x_2 \leq 30 \\ -7x_1 + 12x_2 \leq 84 \\ x_2 \leq 9 \\ 19x_1 + 14x_2 \leq 266 \\ x_1 \leq 10 \\ 4x_1 - 7x_2 \leq 28 \\ x_1 \geq 0, x_2 \geq 0 \end{cases} \end{aligned} \quad [1.118]$$

- classify this optimization problem;
- write the Lagrange formulation of this problem;
- model geometrically all functions (objective and constraints);
- find the optimal solution.

SOLUTION.–

The classification of this optimization problem is a constrained, linear, single-objective problem.

The Lagrange formulation is then written for the constrained optimization problem, where its general form is expressed as follows:

$$\begin{aligned} \min & \quad :f(\mathbf{x}) \\ \text{subject to } & :h_i(\mathbf{x}) = 0 \\ \text{and} & \quad :g_j(\mathbf{x}) \leq 0 \end{aligned} \quad [1.119]$$

Hence, the problem being studied here can be reformulated into the following form:

$$\begin{aligned} \min f(\mathbf{x}) &= -3x_1 - x_2, \\ \text{subject to } &\begin{cases} -6x_1 + 5x_2 - 30 \leq 0 \\ -7x_1 + 12x_2 - 84 \leq 0 \\ x_2 - 9 \leq 0 \\ 19x_1 + 14x_2 - 266 \leq 0 \\ x_1 - 10 \leq 0 \\ 4x_1 - 7x_2 - 28 \leq 0 \\ -x_1 \leq 0, -x_2 \leq 0 \end{cases} \end{aligned} \quad [1.120]$$

The constraints are inequality constraints. They are expressed as follows:

$$\begin{aligned} g_1(x) &= -6x_1 + 5x_2 - 30 \leq 0 \\ g_2(x) &= -7x_1 + 12x_2 - 84 \leq 0 \\ g_3(x) &= x_2 - 9 \leq 0 \\ g_4(x) &= 19x_1 + 14x_2 - 266 \leq 0 \\ g_5(x) &= x_1 - 10 \leq 0 \\ g_6(x) &= 4x_1 - 7x_2 - 28 \leq 0 \\ g_7(x) &= -x_1 \leq 0 \\ g_8(x) &= -x_2 \leq 0 \end{aligned} \quad [1.121]$$

To model this problem geometrically, we model all functions as straight lines. The intersection of the first straight line with the Cartesian axes gives:

$$g_1(x) = -6x_1 + 5x_2 - 30 = 0 \Rightarrow \begin{Bmatrix} P_1(0,6) \\ P_2(-5,0) \end{Bmatrix} \quad [1.122]$$

The intersection of the second straight line with the Cartesian axes gives:

$$g_2(x) = -7x_1 + 12x_2 - 84 = 0 \Rightarrow \begin{Bmatrix} P_1(0,7) \\ P_2(-12,0) \end{Bmatrix} \quad [1.123]$$

The third constraint $g_3(x) = x_2 - 9 = 0$ is parallel to the x_1 axis and the intersection is at the point $P(0,9)$. The intersection of the fourth straight line with the Cartesian axes gives:

$$g_4(x) = 19x_1 + 14x_2 - 266 = 0 \Rightarrow \left\{ \begin{array}{l} P_1(0,19) \\ P_2(14,0) \end{array} \right\} \quad [1.124]$$

The fifth constraint $g_5(x) = x_1 - 10 = 0$ is parallel to the x_2 axis and the intersection is at the point $P(10,0)$. The intersection of the sixth straight line with the Cartesian axes gives:

$$g_6(x) = 4x_1 - 7x_2 - 28 = 0 \Rightarrow \left\{ \begin{array}{l} P_1(0,-4) \\ P_2(7,0) \end{array} \right\} \quad [1.125]$$

The seventh constraint $g_7(x) = -x_1 = 0$ coincides with the x_2 axis and the eighth constraint $g_8(x) = -x_2 = 0$ coincides with the x_1 axis.

To model the iso-values of the objective $f(\mathbf{x}) = -3x_1 - x_2$, we consider several straight lines (several levels). The intersection of the first straight line with the Cartesian axes gives:

$$f(x) = -3x_1 - x_2 = 0 \Rightarrow \left\{ \begin{array}{l} P_1(0,0) \\ P_2(1,-3) \end{array} \right\} \quad [1.126]$$

The intersection of the second straight line with the Cartesian axes gives:

$$f(x) = -3x_1 - x_2 = 1 \Rightarrow \left\{ \begin{array}{l} P_1(0,-1) \\ P_2(-\frac{1}{3},0) \end{array} \right\} \quad [1.127]$$

Figure 1.29 shows the point of the optimal solution $\mathbf{x}^* = (10,5.4)$ where the maximal value of the objective is $f(\mathbf{x}^*) = -35.4$.

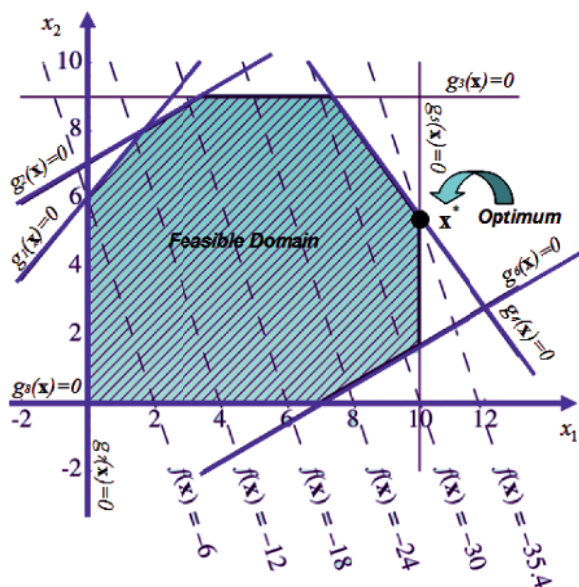


Figure 1.29. Geometrical modeling of the optimal point

1.4.5.2.2. Optimality criteria method

The optimality criteria (OC) method uses the first-order derivatives of the Lagrange formulation. The necessary first-order derivative conditions giving the critical points are written as follows:

$$\frac{\partial L(\mathbf{x}, \lambda, \mu)}{\partial \mathbf{x}} = \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} + \sum_{j=1}^j \lambda_j \frac{\partial h_j(\mathbf{x})}{\partial \mathbf{x}} + \sum_{k=1}^k \mu_k \frac{\partial g_k(\mathbf{x})}{\partial \mathbf{x}} = 0 \quad [1.128]$$

$$\frac{\partial L(\mathbf{x}, \lambda, \mu)}{\partial \lambda} = h_j(\mathbf{x}) = 0 \quad [1.129]$$

$$\frac{\partial L(\mathbf{x}, \lambda, \mu)}{\partial \mu} = g_k(\mathbf{x}) = 0 \quad [1.130]$$

The solution of this problem leads to an optimum which is local and can be global.

ILLUSTRATIVE EXAMPLE 1.6.–

Consider a constrained optimization problem of the following form:

$$\begin{aligned} \min \quad & f(\mathbf{x}) = x_1^2 + x_1x_2, \\ \text{subject to:} \quad & g(\mathbf{x}) = -x_1^2x_2 + 300/\pi \leq 0, \\ & : x_i \geq 0, i = 1, 2. \end{aligned} \quad [1.131]$$

- classify the optimization problem;
- find geometrically the optimal solution;
- find the minimal value using the optimality criteria method.

SOLUTION.–

The classification of this optimization problem is a constrained, nonlinear and single-objective problem.

To model this problem geometrically, we start with the iso-values of the objective function. For the straight line $f(\mathbf{x}) = x_1^2 + x_1x_2 = 10$, we obtain the following points: $P_1(1,9)$, $P_2(5,-3)$ and $P_3(10,-9)$. Next, for the straight line $f(\mathbf{x}) = x_1^2 + x_1x_2 = 20$, we obtain the following points: $P_1(1,19)$, $P_2(5,-1)$ and $P_3(10,-8)$.

To model the first constraint $g_1(\mathbf{x}) = -x_1^2x_2 + 300/\pi = 0$, we obtain the following points: $P_1(10,0.95)$, $P_2(10,3.09)$ and $P_3(15,0.42)$ which corresponds to objective function values of: $f_1(\mathbf{x}) = 109.54$, $f_2(\mathbf{x}) = 40.44$ and $f_3(\mathbf{x}) = 232.35$. The second constraint $g_2(x) = -x_1 = 0$ coincides with the x_2 axis and the third constraint $g_3(x) = -x_2 = 0$ coincides with the x_1 axis. Figure 1.30 shows a representation of this optimization problem.

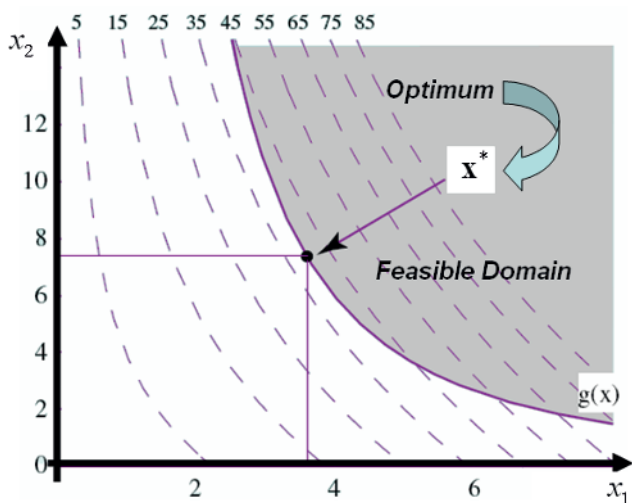


Figure 1.30. Geometrical modeling of the studied optimization problem

We find that the problem is nonlinear, meaning that an iterative method is required to find the optimal solution.

To use the optimality criteria method, we rewrite the constraints considering the standard forms:

$$\begin{aligned}
 g_1(x) &= -x_1^2 \cdot x_2 + \frac{300}{\pi} \leq 0 \\
 g_2(x) &= -x_1 \leq 0 \\
 g_3(x) &= -x_2 \leq 0
 \end{aligned}
 \tag{1.132}$$

The Lagrange formulation can be written using the following form:

$$L = x_1^2 + x_1 \cdot x_2 + \mu_1 \left(-x_1^2 x_2 + \frac{300}{\pi} \right) + \mu_2 (-x_1) + \mu_3 (-x_2)
 \tag{1.133}$$

By differentiating this formulation, we obtain:

$$\frac{\partial L}{\partial x_1} = 2x_1 + x_2 - 2\mu_1 x_1 x_2 - \mu_2 = 0
 \tag{1.134}$$

$$\frac{\partial L}{\partial x_2} = x_1 - \mu_1 x_1^2 - \mu_3 = 0 \quad [1.135]$$

$$\frac{\partial L}{\partial \mu_1} = -x_1^2 x_2 + \frac{300}{\pi} = 0 \quad [1.136]$$

$$\frac{\partial L}{\partial \mu_2} = -x_1 = 0 \quad [1.137]$$

$$\frac{\partial L}{\partial \mu_3} = -x_2 = 0 \quad [1.138]$$

Assuming that the two variables are not null ($x_1 \neq 0$ and $x_2 \neq 0$), we obtain ($\mu_2 = \mu_3 = 0$). Equation [1.134] becomes:

$$2x_1 + x_2 - 2\mu_1 x_1 x_2 = 0 \quad [1.139]$$

which leads to:

$$\mu_1 = \frac{2x_1 + x_2}{2x_1 x_2} \quad [1.140]$$

When substituting this result into equation [1.135], we obtain:

$$x_1 - \mu_1 x_1^2 = 0 \Rightarrow x_1 - \left(\frac{2x_1 + x_2}{2x_1 x_2} \right) x_1^2 = 0 \Rightarrow x_2 = 2x_1 \quad [1.141]$$

which leads to:

$$x_2 = 2x_1 \quad [1.142]$$

When substituting this result into equation [1.136], we obtain:

$$-x_1^2 x_2 + \frac{300}{\pi} = 0 \Rightarrow -x_1^2 (2x_1) + \frac{300}{\pi} = 0 \quad [1.143]$$

which leads to the optimal solution $x_1 = 3.627$ and $x_2 = 7.2556$. The value of the objective function is then $f(\mathbf{x}^*) = 39.47$. Figure 1.30 shows the geometrical interpretation of this optimization problem.

ILLUSTRATIVE EXAMPLE 1.7.—

Consider an optimization problem of the following form:

$$\begin{aligned} \min \quad & :Cost(b, h) = 12b + 10h - 2b^2 - bh - h^2 \\ \text{subject to:} & b + h \geq 4 \end{aligned} \quad [1.144]$$

- classify the optimization problem;
- find geometrically the optimal solution;
- find the minimal value using the optimality criteria method.

SOLUTION.—

The classification of this optimization problem is a constrained, nonlinear and single-objective problem.

To geometrically model this problem, we rewrite the inequality constraint in the standard form:

$$g_1(x) = 4 - b - h \leq 0 \quad [1.145]$$

The boundary of this constraint corresponds to a straight line. The intersection of this straight line with the Cartesian axes gives:

$$g_1(x) = 4 - b - h = 0 \Rightarrow \begin{cases} P_1(0, 4) \\ P_2(4, 0) \end{cases} \quad [1.146]$$

Next, we model the iso-values of the objective function (several levels). At the level $Cost(b, h) = 12b + 10h - 2b^2 - bh - h^2 = 0$, the intersection with the horizontal axis gives:

$$b = 0 \Rightarrow 10h - h^2 = 0 \Rightarrow h = 0, h = 10 \quad [1.147]$$

The intersection with the vertical axis gives:

$$h = 0 \Rightarrow 12b - 2b^2 = 0 \Rightarrow b = 0, b = 6 \quad [1.148]$$

At the level $Cost(b, h) = 12b + 10h - 2b^2 - bh - h^2 = 10$, the intersection with the horizontal axis gives:

$$b = 0 \Rightarrow 10h - h^2 = 10 \Rightarrow h = 1.127, h = 8.87 \quad [1.149]$$

The intersection with the vertical axis gives:

$$h = 0 \Rightarrow 12b - 2b^2 = 0 \Rightarrow b = 1, b = 5 \quad [1.150]$$

At the level $Cost(b, h) = 12b + 10h - 2b^2 - bh - h^2 = 20$, the intersection with the horizontal axis gives:

$$b = 0 \Rightarrow 10h - h^2 = 20 \Rightarrow h = 2.76, h = 7.23 \quad [1.151]$$

The intersection with the vertical axis gives:

$$b = 1 \Rightarrow 12 + 10h - 2 - h - h^2 = 20 \Rightarrow h = 1.29, h = 7.7 \quad [1.152]$$

which leads to the optimal solution $b = 1.5$ and $h = 2.5$. The value of the objective function is then $f(b, h) = 28.5$. Figure 1.31 shows the geometrical interpretation of this optimization problem.

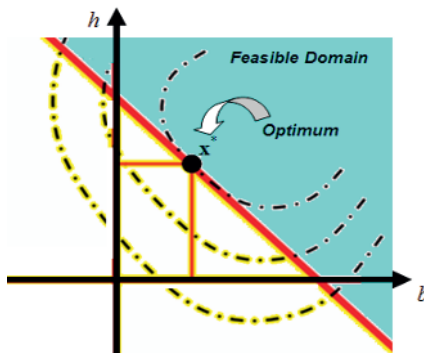


Figure 1.31. Geometric model of the optimization problem

The Lagrange formulation can be written using the following form:

$$L(b, h, \mu) = 12b + 10h - 2b^2 - bh - h^2 + \mu[4 - b - h] \quad [1.153]$$

When differentiating this formulation, we obtain:

$$\frac{\partial L}{\partial b} = 0 \Rightarrow 12 - 4b - h - \mu = 0 \quad [1.154]$$

$$\frac{\partial L}{\partial h} = 0 \Rightarrow 10 - b - 2h - \mu = 0 \quad [1.155]$$

$$\frac{\partial L}{\partial \mu} = 0 \Rightarrow 4 - b - h = 0 \quad [1.156]$$

We have three linear equations with three unknowns. The analytic solution gives $b = 1.5$, $h = 2.5$ and $\mu = 3.5$. The minimal value of the objective function is thus $\min Cost = 28.5$.

ILLUSTRATIVE EXAMPLE 1.8.–

Consider an optimization problem in the following form:

$$\begin{aligned} \min \quad & : f(\mathbf{x}) = 2x_1^2 - 2x_1 + \frac{1}{2}x_2^2 - 3x_2 \\ \text{subject to} \quad & : -(x_1 - 1)^2 - x_2^2 + 2x_2 \geq 1 \\ \text{and} \quad & : x_1 \geq 0, x_2 \geq 0 \end{aligned} \quad [1.157]$$

- classify the optimization problem;
- find the minimal value using the optimality criteria method.

SOLUTION.–

The classification of this optimization problem is a constrained, nonlinear, single-objective problem.

To use the optimality criteria method, we rewrite the constraints using the standard form:

$$\begin{aligned} g_1(\mathbf{x}) &= (x_1 - 1)^2 + x_2^2 - 2x_1 + 1 \leq 0 \\ g_2(x) &= -x_1 \leq 0 \\ g_3(x) &= -x_2 \leq 0 \end{aligned} \quad [1.158]$$

The Lagrange formulation can be written as follows:

$$L = 2x_1^2 - 2x_1 + \frac{1}{2}x_2^2 - 3x_2 + \mu_1 [(x_1 - 1)^2 + x_2^2 - 2x_1 + 1] + \mu_2(-x_1) + \mu_3(-x_2) \quad [1.159]$$

When differentiating this formulation, we obtain:

$$\frac{dL}{dx_1} = 4x_1 - 2 + 2\mu_1(x_1 - 1) - 2\mu_1 - \mu_2 = 0 \quad [1.160]$$

$$\frac{dL}{dx_2} = x_2 - 3 + 2\mu_1 x_2 - \mu_3 = 0 \quad [1.161]$$

$$\frac{dL}{d\mu_1} = (x_1 - 1)^2 + x_2^2 - 2x_1 + 1 = 0 \quad [1.162]$$

$$\frac{\partial L}{\partial \mu_2} = -x_1 = 0 \quad [1.163]$$

$$\frac{\partial L}{\partial \mu_3} = -x_2 = 0 \quad [1.164]$$

Assuming that the two variables are not null ($x_1 \neq 0$ and $x_2 \neq 0$), we obtain ($\mu_2 = \mu_3 = 0$). Equation [1.160] becomes:

$$4x_1 - 2 + 2\mu_1(x_1 - 2) = 0 \quad [1.165]$$

which leads to:

$$\mu_1 = \frac{2 - 4x_1}{2(x_1 - 2)} \quad [1.166]$$

When substituting this result into equation [1.161], we obtain:

$$x_2 - 3 + 2\mu_1 x_2 = 0 \quad [1.167]$$

which leads to:

$$x_2 = \sqrt{2x_1 - 1 - (x_1 - 1)^2} \quad [1.168]$$

When substituting this result into equation [1.162], we obtain:

$$\sqrt{2x_1 - 1 - (x_1 - 1)^2} - 3 + 2 \left(\frac{2 - 4x_1}{2(x_1 - 2)} \right) \sqrt{2x_1 - 1 - (x_1 - 1)^2} = 0 \quad [1.169]$$

which leads to the optimal solution $x_1 = 1$, $x_2 = 1$ and $\mu_1 = 1$. The geometric solution is only effective for bivariable problems with linear functions.

1.5. Sensitivity analysis

1.5.1. Importance of sensitivity

Sensitivity analysis of a mathematical model consists of studying the variation impact of the input parameters on the output parameters of the model. The sensitivity of a function (or indeed the derivative of this function) with respect to several variables gives the influence of each variable on the studied function. The sensitivity calculation can be explicit or implicit [KHA 11].

ILLUSTRATIVE EXAMPLE 1.9.—

Figure 1.32 shows a cantilever beam of a rectangular cross-section ($b \times h$) subjected to a static force F and fixed at the other end.

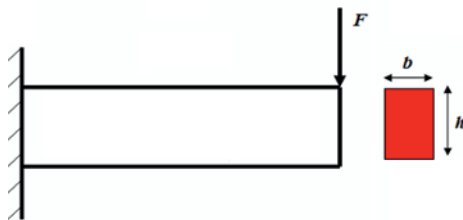


Figure 1.32. Simple model of a cantilever beam

The maximal mechanical stress can be found at the end of the beam and can be mathematically calculated as follows:

$$\sigma_{\max} = \frac{M_{\max}}{I} \times \frac{h}{2} \quad [1.170]$$

where I is the inertia moment for a rectangular cross-section and can be calculated using the following relationship:

$$I = \frac{b \cdot h^3}{12} \quad [1.171]$$

The derivatives of the maximal mechanical stress with respect to the two dimensions show that the beam height has much more of an effect than the beam width ($\partial I / \partial h \gg \partial I / \partial b$). In this example, we have an explicit model because the derivative can be calculated analytically. In contrast, Figure 1.33 shows the same beam, but with transverse holes drilled through it, which leads to an infinite number of cross-sections.

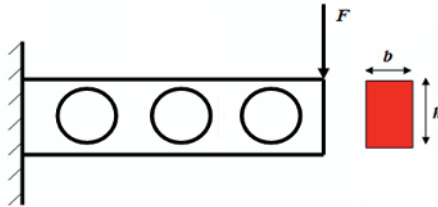


Figure 1.33. *Implicit model of a cantilever beam*

In order to calculate the derivative of this implicit model, we have to use numerical methods to carry out the sensitivity analysis.

1.5.2. Sensitivity methods

Sensitivity analysis is an important tool during the development, construction or use of a mathematical model. In fact, when studying how a model responds to variations in its input variables, sensitivity analysis can answer a number of questions. Sensitivity analysis can

be carried out in three ways: numerically, analytically and semi-analytically [KHA 03]. We are interested in the numerical method of finite differences, which is very simple to implement.

Using the finite difference (FD) method, we calculate the first derivative $df(x_i)/dx_i$ with the following techniques:

1) Forward finite difference (FFD):

$$\frac{df(x_i)}{dx_i} \cong \left[\frac{\Delta f(x_i)}{\Delta x_i} \right]_{FFD} = \frac{f(x_i + \Delta x_i) - f(x_i)}{\Delta x_i} \quad [1.172]$$

2) Backward finite difference (BFD):

$$\frac{df(x_i)}{dx_i} \cong \left[\frac{\Delta f(x_i)}{\Delta x_i} \right]_{BFD} = \frac{f(x_i) - f(x_i - \Delta x_i)}{\Delta x_i} \quad [1.173]$$

3) Central finite difference (CFD):

$$\frac{df(x_i)}{dx_i} \cong \left[\frac{\Delta f(x_i)}{\Delta x_i} \right]_{CFD} = \frac{f(x_i + \Delta x_i) - f(x_i - \Delta x_i)}{2\Delta x_i} \quad [1.174]$$

The choice of the increment Δx_i to achieve a good accuracy is difficult. Figure 1.34 shows that the value of the derivative varies as a function of Δx_i .

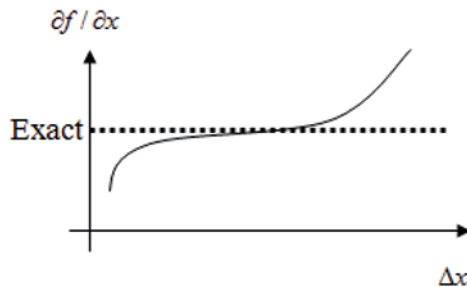


Figure 1.34. Numerical derivative as a function of the increment

ILLUSTRATIVE EXAMPLE 1.10.–

Considering a function $f(x) = 4x^2 - 8x + 13$, we test the finite difference precision by calculating the sensitivity or the derivatives of this function at the point $x = 2.5$.

Using the FFD technique, the change of Δx_i can lead to the exact value of the derivative $\partial f(x) / \partial x$ (Figure 1.35).

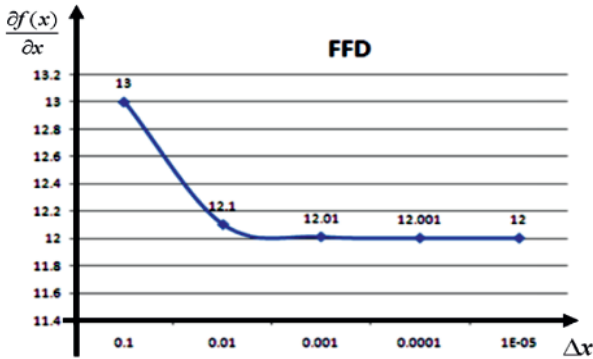


Figure 1.35. Precision curve using FFD technique

Using the BFD technique, the change of Δx_i can lead to the exact value of the derivative $\partial f(x) / \partial x$ (Figure 1.36).

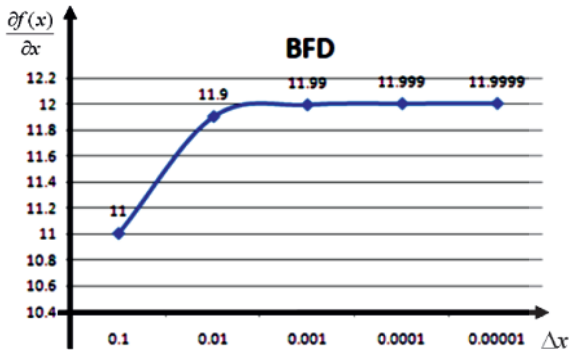


Figure 1.36. Precision curve using BFD technique

Using the CFD technique, the change of Δx_i can lead to the exact value of the derivative $\partial f(x) / \partial x$ (Figure 1.37).

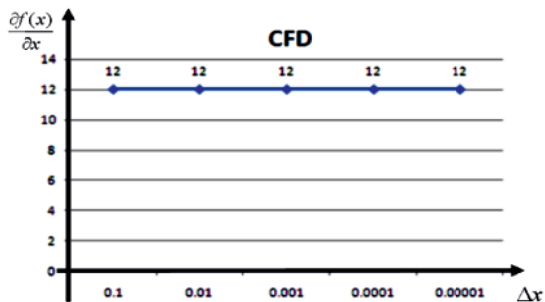


Figure 1.37. Precision curve using CFD technique

We find that the CFD technique gives exact values for all values of the increment Δx_i . Figure 1.38 shows the algorithm for finite difference calculations of derivatives with high precision, ε .

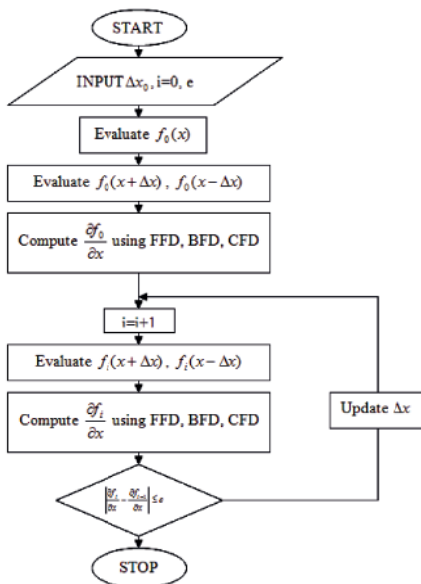


Figure 1.38. Algorithm of precision, ε , with finite difference methods

Furthermore, considering the precision advantage of the CFD technique, we can also calculate the second derivative as a function of a single variable using the following formula:

$$\frac{d^2 f}{dx_i^2} = \frac{f(x_i + 2\Delta x_i) - 2f(x_i + \Delta x_i) + f(x_i)}{\Delta x_i^2} \quad [1.175]$$

In the same way, we can calculate the second derivative as a function of two variables as follows:

$$\begin{aligned} \frac{d^2 f}{dx_i dx_j} &= \dots \\ &= \frac{f(x_i + \Delta x_i, x_j + \Delta x_j) - f(x_i + \Delta x_i, x_j) - f(x_i, x_j + \Delta x_j) + f(x_i, x_j)}{\Delta x_i \Delta x_j} \end{aligned} \quad [1.176]$$

The equations for the first-order derivatives can be used in first-order optimization methods (DGM and CGM). In contrast, the equations for the second-order derivatives can be used in the second-order optimization methods (NM and MNM) [KHA 11].

1.6. Conclusion

In this chapter, several mathematical and numerical tools have been presented as basic concepts to be used in the following chapters. Geometric models in biomechanics are very complicated and require a numerical simulation (for example, FEM) to solve the studied problem. Understanding the optimization technology is an essential stage to apply reliability analysis in biomechanics. Additionally, sensitivity analysis can be carried out during the optimization process and reliability analysis in order to identify the influence of input parameters on the output responses.

