CHAPTER 1

INTRODUCTION

1. Introduction

Because of the fast development in computer technology and its applications, there is a great deal of interest in making use of applied mathematics and in developing new techniques to meet new situations. Numerical Analysis is such an area, particularly iteration techniques. These are old and well-known mathematical tools with widespread applications in both theoretical and applied work. However their mathematical counterparts, stochastic approximations, are of relatively recent origin and in a state of rapid growth.

Professor H. Hotelling discussed many ideas of stochastic approximations in his paper of 1941 [46] and relevant results have been given by Friedman and Savage [38] and others. But Robbins and Monro [63] in their pioneer paper gave a formal mathematical treatment of this field and proved many interesting results. Since then many papers on the subject have appeared in theoretical and applied journals, indicating its usefulness and growing importance.

In this chapter in order to motivate the subject, a number of practical problems are stated as illustrative examples. Some interesting examples are also given in the chapter of applications. A method of stochastic approximation is defined, and is then compared with another sequential method the so-called up-and-down method, and with iterative techniques of Numerical Analysis. Some of its merits and demerits which indicate situations where stochastic approximation can be exploited with advantage are appended. In the last section of this chapter we summarize the main results of each chapter.

2. Illustrative examples

(*a*) It is known that hardness of copper–iron alloy is influenced by the length of time the alloy is aged at 500 °C. Let x be this length of time and $Y(x)$ be the hardness of the alloy, the problem is to find the values of x which can give an alloy of a given average hardness α. It is a well-known fact that hardness varies from alloy to alloy.

(*b*) Let us consider the sensitivity of explosive to shock. A common method is to drop a known weight of some explosive mixture from a given height, some will explode, others will not. Each specimen has a critical height, the problem is to determine this height.

(*c*) In testing insecticides, one may be confronted with the problem of determining the critical dose for a given quantitative response.

(*d*) Let us consider a plot where x lbs of fertilizer is applied, and $Y(x)$ lbs of corn is produced. The yield will probably be small if a smaller amount of fertilizer is used, but also if too much is used. Somewhere in between the maximum yield will be achieved. Yield will, of course, vary from year to year even though x remains the same.

3. Stochastic approximations

The situations discussed in (*a*), (*b*) and (*c*) can be formalized mathematically in the following manner. In the region of experimentation an experimenter chooses arbitrarily a value x_1, conducts an experiment and observes the value $y(x_1)$ of the random variable $Y(x_1)$ with expectation $M(x) = E\{Y(x_1)\}$, where E denotes mathematical expectation and M is some increasing function of unknown form. He chooses also a sequence of positive numbers a_n which decreases with n. For example, he can choose $a_n = c/n$, where c is any positive real number. His problem is to determine the value of θ such that $M(\theta) = \alpha$. He sets up the following recursive relation in order to pick a value of x for his next experiment.

$$x_{n+1} = x_n - \frac{c}{n}[y(x_n) - \alpha]. \tag{1}$$

Suppose he has already conducted the nth experiment and that as a result he knows x_n and the value of $y(x_n)$ Then using (1) he can determine what value of x he should use in the $(n+1)$th experiment. Let us examine this recursive relation. For simplicity let $\alpha = 0$. Then (1) reduces to the form

$$x_{n+1} = x_n - \frac{c}{n} y(x_n). \tag{2}$$

If the value of $y(x_n) > 0$ then $x_{n+1} < x_n$ and if $y(x_n) < 0$ then $x_{n+1} > x_n$. This seems to be reasonable because one is interested in solving $M(\theta) = 0$. If $y(x_n)$ is positive then one should decrease the value of x for the $(n+1)$th stage of experimentation, and vice versa. In Chapter 2 conditions under which the sequence $\{x_n\}$ converges in mean square and with probability one to the solution θ are stated. For the situation (*d*) refer to Chapter 3 for a method of locating the maximum of the regression function $M(x)$.

The up-and-down method, another sequential method, is a relevant competitor to a stochastic approximation method.

4. Up-and-down method

Consider such situations as (*a*), (*b*) and (*c*). Suppose now an experimenter chooses x_1 arbitrarily and also a constant d which is approximately equal to the standard deviation of the random variable. Again he is interested in solving the equation $M(x) = \alpha$. He tests a single subject at any given time. If at the nth step in the process the stimulus is at level x_n, the sequential rule is that the $(n+1)$th test be made at level

$$X_{n+1} = \begin{cases} X_n + d & \text{if there is no response at } X_n, \\ X_n - d & \text{if there is response at } X_n, \end{cases} \tag{1}$$

when the experiment is terminated at some chosen value n. An essential difference between the up-and-down method and the stochastic approximation method is that for the up-and-down method the value of x is changed by a fixed amount d in the direction dictated by the experiment. In some experimental situation it is feasible only to change the value of x by a fixed amount d. An approach to the problem is that of Probit Analysis. A choice of a method to be employed is determined by practical limitations

5. Newton–Raphson method

We now define the Newton–Raphson method, an iterative technique of Numerical Analysis, and discuss its comparison with a stochastic approximation method.

Let M be a function from the real interval $I = [a, b]$ to I, whose form is unknown. The problem is to solve the equation $M(x) = \alpha$. One can do this by the following iteration techniques. Choose x_1 arbitrarily in the interval I and use the following recursive scheme to generate a sequence which will converge to the desired solution.

$$x_{n+1} = x_n - [M'(x_n)]^{-1}[M(x_n) - \alpha], \tag{1}$$

where $M'(x_n)$ is the derivative of M at $x = x_n$. Appendix 1 gives the appropriate conditions under which a solution exists. (1) can be written as follows:

$$x_{n+1} = x_n - a_n[M(x_n) - \alpha], \tag{2}$$

where $a_n = [M'(x_n)]^{-1}$ which is assumed to exist and to be bounded. From equation (1) of §1.3,

$$\left.\begin{aligned} X_{n+1} &= X_n - a_n[Y(X_n) - \alpha], \\ X_{n+1} &= X_n - a_n[M(X_n) - \alpha] - a_n[Y(X_n) - M(X_n)]. \end{aligned}\right\} \tag{3}$$

Equation (3) looks like (2) but with the additional element $-a_n[Y(x_n) - M(x_n)]$ (which may be described as 'noise' arising from the fact that $M(x_n)$ is not exactly observable). Thus in order to have a solution we will have to assume all the conditions of Appendix 1. That is, M will have to be monotone or continuous on the interval $[a, b]$, and satisfy the Lipschitz condition there. In addition we will have to assume conditions under which the 'noise' $-a[Y(x_n) - M(x_n)]$ should disappear as the number of iterations increase. That is essentially what we shall do in subsequent chapters.

6. Applications

We have seen in §1.2 that there are a number of applied problems where stochastic approximation could be employed. But these problems can be solved by other statistical methods, for example, in some cases the method of least squares may be used.

Kushner [55] has concluded that the least-squares method is superior to the stochastic-approximation method after discussing the efficiency of the two methods. The main advantage with the stochastic-approximation method is that one need not know about the input of the system, all one needs to know is the output which is easily available in practice. Furthermore, it is unnecessary to know the form of the regression function or to estimate unknown parameters. Thus stochastic approximation is a non-parametric technique which quite often generates a non-Markov stochastic process.

There are three main problems associated with stochastic-approximation procedure. First, one will be interested in the convergence and mode of convergence of the sequence generated by the method to the desired solution of the equation. Secondly, one would like to know the asymptotic distribution of the sequence. Finally, since stochastic approximation is a sequential procedure, one will be interested to know an optimum stopping rule for a given situation. The first problem is tackled in Chapters 2, 3, 5, and 7, the second in Chapter 6. It appears that these two problems have been answered satisfactorily, but the problem of optimum sequential stopping rules has hardly been attempted. A paper pertaining to the subject is that of Farrell [35].

7. Summary

In Chapter 2 the Robbins–Monro method is described for a particular applied problem of response-no-response analysis. This has motivated the subject of stochastic approximation and reflected what is involved mathematically. Then a general one-dimensional stochastic approximation is investigated. It is shown that when one has some knowledge of the process one can relax conditions. For example, if it is known only that the stochastic-approximation sequence is regular, the conditions imposed on the iterating coefficients can be relaxed. A small sample theory is discussed and comparison is made with the asymptotic one. Then many modifications of a general case are mentioned which have revealing effect on the stochastic-approximation procedures.

Chapter 3 discusses a method of Kiefer and Wolfowitz for determining the location of a maximum of a regression function, and singles out the optimum choice of iterating coefficients. A unified treatment of the subject of Chapters 2 and 3 is given and a procedure for obtaining the location of an inflection point is stated. For a simple regression model, a stochastic-approximation technique is exploited with advantage.

Chapter 4 shows how a method of stochastic approximation can be used in a control problem and its difference from the conventional procedure. Then a problem of pharmocology is discussed. Its application to a reliability situation indicates how such a method is effective in measuring information. Its uses in problems of bioassay are investigated.

In Chapter 5 a multivariate stochastic-approximation procedure is introduced and its utility in the investigation of a kinetic model of pharmocology is discussed.

Chapter 6 deals with the problem of asymptotic distribution and exploits a method of moments and a characteristic function method. An application to the construction of confidence interval is indicated.

In Chapter 7 the techniques of stochastic approximation for continuous random processes are dealt with and their utility for analogue computers is stated. Their applications to a control problem, and a filter problem are discussed.

In Chapter 8 an 'up-and-down' method is investigated and its application to 'Rankits' is shown. Small sample and non-parametric up-and-down methods are appended.

Appendices on the subjects of iterative techniques, limit theorems and inequalities are also added. These are mathematical tools which are exploited in order to develop the theory of stochastic approximation.

The problems at the end of each chapter provide additional information which is obtainable from the references.

REMARK. It will be clear from the context of the material whether we are dealing with a random variable or just its numerical value.

CHAPTER 2

THE ROBBINS–MONRO METHOD

1. Introduction

In this chapter the mathematical aspects of the Robbins–Monro method are dealt with. First, response–no-response analysis is considered; this throws light on the mathematical subtleties involved. Secondly, a general result due to Dvoretzky is proved; this has many modifications, which reveal many ways to economize the iterative procedures.

If one has a regular process, then one can relax the conditions on the iterative coefficients. This is discussed in §2.4. In practice one generally deals with small sample theory and it is interesting to see its relation to large sample theory, which is discussed in §2.5.

2. Response–no-response analysis

In this section a simple case of the Robbins–Monro method is considered. This illustrates the mathematical techniques involved in proving a general result and prepares the reader for what he may expect in this chapter.

In many problems of bioassay and applied statistics one obtains response–no-response data from an experiment. For example in in testing insecticides one observes whether or not an insect responds to a certain dose. Thus the problem is to determine the critical dose for a given quantitative response. Mathematically the problem can be formulated in the following way.

Let Z be a random variable with distribution function M. If x is a real number and $Y(x)$ a random variable such that

$$Y(x) = 1 \quad \text{if } Z \leqslant x$$
$$= 0 \quad \text{if } Z > x$$

then
$$P[Y(x) = 1] = P[Z \leqslant x] = M(x),$$
$$P[Y(x) = 0] = P[Z > x] = 1 - M(x),$$
$$E[Y(x)] = 1.M(x) + 0.(1 - M(x)) = M(x).$$

Now $Y(x)$ is the observable response to a dose x. The problem is to determine the value of x for a given quantitative response α. This can be done as described in the following theorem.

THEOREM 1. *Let M be a distribution function and α a real number such that there is a real number θ giving $M(\theta) = \alpha$; let M be differentiable at θ and have $M'(\theta) > 0$. Let x_1 be a real number and n be a positive integer. Let*

$$X_{n+1} = X_n - \frac{1}{n}(Y_n - \alpha), \tag{1}$$

where Y_n is a random variable such that

$$P[Y_n = 1 | X_1 X_2, \ldots, X_n, \; Y_1, \ldots, Y_{n-1}] = M(X_n),$$

$$P[Y_n = 0 | X_1 X_2, \ldots, X_n, \; Y_1, \ldots, Y_{n-1}] = 1 - M(X_n).$$

Then $\lim_{n\to\infty} E(X_n - \theta)^2 = 0$, so that random variable sequence $\{X_n\}$ converges to θ in mean square and hence in probability.

Proof. Let $\xi_n = E(X_n - \theta)^2$ we want to show that $\lim_{n\to\infty} \xi_n = 0$. From (1) we have

$$X_{n+1} - \theta = X_n - \theta - \frac{1}{n}(Y_n - \alpha).$$

Therefore

$$E(X_{n+1} - \theta)^2 = E(X_n - \theta)^2 - \frac{2}{n} E[(X_n - \theta)(Y_n - \alpha)] + \frac{1}{n^2} E(Y_n - \alpha)^2.$$

Let
$$d_n = E[(X_n - \theta)(Y_n - \alpha)],$$
$$e_n = E(Y_n - \alpha)^2,$$

then
$$\xi_{n+1} = \xi_n - \frac{2}{n} d_n + \frac{e_n}{n^2},$$

$$\sum_{j=1}^{n} (\xi_{j+1} - \xi_j) = -2 \sum_1^n \frac{d_j}{j} + \sum_1^n \frac{e_j}{j^2},$$

$$\xi_{n+1} - \xi_1 = -2 \sum_1^n \frac{d_j}{j} + \sum_1^n \frac{e_j}{j^2}.$$

Since
$$0 \leqslant e_n = E(Y_n - \alpha)^2 \leqslant 1, \sum_1^n \frac{e_j}{j^2}$$

is non-decreasing and bounded, and

$$\sum_{j=1}^{\infty} \frac{e_j}{j^2}$$

converges, because $\sum_1^\infty \frac{1}{j^2} = \frac{\pi^2}{6}$,

$$\begin{aligned} d_n &= E[(X_n - \theta)(Y_n - \alpha)] \\ &= E\{E[(X_n - \theta)(y_n - \alpha) | X_1, \ldots, X_n, Y_1, \ldots, Y_{n-1}]\} \\ &= E[(X_n - \theta)(M(X_n) - \alpha)] \geqslant 0 \end{aligned}$$

since $(X - \theta)(M(X) - \alpha) \geqslant 0$ for all X.

Hence $2\sum_1^n \frac{d_j}{j} = \xi_1 - \xi_{n+1} + \sum_1^n \frac{e_j}{j} \leqslant \xi_1 + \sum_{j=1}^{\infty} \frac{e_j}{j^2}$

and thus $\sum_1^n \frac{d_j}{j}$

is bounded non-decreasing, which implies that

$$\sum_1^\infty \frac{d_j}{j}$$

converges. Therefore

$$\lim_{n\to\infty} \xi_{n+1} = \xi_1 - 2\sum_1^\infty \frac{d_j}{j} + \sum_1^\infty \frac{e_j}{j^2} = \xi$$

exists. We want to show that $\xi = 0$.

Suppose there is a real number sequence $\{k_n\}$ such that

$$\left.\begin{array}{ll} (1) & k_n \geqslant 0 \\ (2) & d_n \geqslant k_n \xi_n \end{array}\right\} \text{ for all } n,$$

$$(3) \quad \sum_1^\infty \frac{k_n}{n} = \infty \text{ diverges,}$$

then $\xi = 0$. To see this, note that (1) and (2) imply that

$$0 \leqslant \sum_1^\infty \frac{1}{n} k_n \xi_n \leqslant \sum_1^\infty \frac{d_n}{n} < \infty.$$