Global Optimization by Random Perturbation of the Gradient Method with a Fixed Parameter

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Abstract. The paper deals with the global minimization of a differentiable cost function mapping a ball of a finite dimensional Euclidean space into an interval of real numbers. It is established that a suitable random perturbation of the gradient method with a fixed parameter generates a bounded minimizing sequence and leads to a global minimum: the perturbation avoids convergence to local minima. The stated results suggest an algorithm for the numerical approximation of global minima: experiments are performed for the problem of fitting a sum of exponentials to discrete data and to a nonlinear system involving about 5000 variables. The effect of the random perturbation is examined by comparison with the purely deterministic gradient method.

Key words. Global optimization, random perturbations, Monte Carlo methods.

1. Introduction

The article deals with the global minimization of a differentiable cost function J mapping a ball B of a finite dimensional Euclidean space E on an interval of real numbers. Let us recall that the usual deterministic gradient method with a fixed parameter $\mu > 0$ for such a problem reads as follows:

- Select an initial guess $x_0 \in E$;
- Generate a sequence of vectors $\{x_n\}_{n\geq 1} \subset E$, defined by

$$\forall n \geq 0: \quad x_{n+1} = Q(x_n)\,, \tag{1}$$

where

$$Q(x) = x - \mu \nabla J(x) \tag{2}$$

and $\nabla J(x)$ is the gradient of J at the point x.

This method is closely connected to the relaxation procedure for the system of nonlinear equations $\nabla J(x) = 0$: let us set $g_n = |\nabla J(x_n)|$. If $\mu > 0$ is correctly chosen, the behaviour of the sequence $\{g_n\}_{n\geq 0}$ is such that: given $\varepsilon > 0$, we have, for n large enough, $g_n \leq \varepsilon$. However, such a method can fail to find global minima of J. Under general conditions, it can lead to local minima (see, for instance [13] and the references therein). Several modifications of the basic procedure (1) have been considered as multistart, statistical gradient or trajectory methods (see, for instance [10], [12]). More recently, in the frame of the simulated annealing

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procedure, methods which are analogous to (1) but with variable μ and a random perturbation have been considered and results of convergence can be found in the literature (see, for instance [1], [5], [6], [7], [8]). These results suggest an algorithm for the numerical approximation of the global minima of J: roughly speaking, the sequence $\{x_n\}_{n\geq 1}$ is not generated by (1) but by the following random perturbated gradient method

$$\forall n \geq 0: x_{n+1} = Q(x_n) + P_n \,, \tag{3}$$

where P_n is a random perturbation which decreases slowly enough in order to escape from local minima. As previously observed, this procedure is similar but not exactly the same as these which have been studied in the frame of the simulated annealing procedure, since μ remains independent of n. Thus, this last assumption leads to rather straightforward arguments when proving both boundedness and convergence results, further the numerical performing is simplified. In Section 2, the random term P_n is precised. Results about the boundedness and the convergence of the generated sequence $\{x_n\}_{n\geq 1}$ are established in Sections 3 and 4: the connection with global minima of J is considered. Numerical experiments are performed in Section 5: (3) is applied to the problem of fitting a sum of exponentials to discrete data and to a problem involving a great number of variables (about 5000) – a nonlinear set of equations resulting from the discretization of a partial differential equation of mixed type: the effect of the random perturbation is examined by a comparison with (1).

2. Random Perturbation of the Gradient Method

2.1. NOTATION AND ASSUMPTIONS ON DETERMINISTIC VARIABLES

Let $\mu > 0$ be given, $N > 0$ be an integer. We denote by $\mathcal{R}$ (respectively $\mathcal{R}^+$) the real line $]-\infty, +\infty[$ (respectively the set of positive real numbers $]0, +\infty[$, $E = \mathcal{R}^N$, the N-dimensional real Euclidean space. For $x = (x_1, \ldots, x_N) \in E$, we set $|x| = (x_1^2 + \cdots + x_N^2)^{1/2}$ – the Euclidean norm of x. The inner product associated to $|\bullet|$ is denoted by $(\bullet, \bullet)$. The cost function is denoted by J. The assumptions on J are the following:

$$J \text{ is continuously differentiable on } E \,; \tag{4.1}$$

$\exists R_c > 0$ such that:

$$R > R_c \Rightarrow \alpha(R) = \frac{1}{R^2} \inf_{R_c \leq |x| \leq R} (\nabla J(x), x) > 0 \,. \tag{4.2}$$

We consider a ball $B \subset E$ of radius $R > R_c$:

$$B = \{x \in E \mid |x| \leq R\} \,.$$

Assumptions (4.1) and (4.2) imply that

$$R > R_c \Rightarrow \frac{1}{R} \sup_B |\nabla J(x)| \in \mathcal{R}^+ , \tag{4.3}$$

and

$$R > R_c \Rightarrow \inf_B J(x) \in \mathcal{R} . \tag{4.4}$$

We observe that, since J is continuous,

$$\exists x^* \in B: J(x^*) = m \quad \text{with } m = \inf_B J(x) .$$

For $\theta > m$, we denote by S_θ the set

$$S_\theta = \{x \in B \mid m \leqslant J(x) \leqslant \theta\} . \tag{4.5}$$

The hypotheses on J imply also that there exists $\delta > 0$ such that, for all $\theta \in]m, m+\delta[$, both S_θ and $B - S_\theta$ have a strictly positive measure:

$$\text{meas}(S_\theta)\, \text{meas}(B - S_\theta) > 0 . \tag{4.6}$$

These properties are used in the proof of the results stated in the following sections. The proof uses also the notations below:

$$\alpha(R) = \frac{1}{R^2} \inf_{R_c \leqslant |x| \leqslant R} (\nabla J(x), x) ; \tag{5}$$

$$a(R) = \frac{1}{R} \sup_B |\nabla J(x)| ; \tag{6}$$

$$m(R) = \inf_B J(x) ; \tag{7}$$

$$\beta(R) = \sup_{(x,y) \in B^2} |y - Q(x)| . \tag{8}$$

In order to simplify the mathematical expressions, parameter R may be omitted in the expressions above.

2.2. THE RANDOM PERTURBATION

We consider a sequence of real numbers $\{\lambda_n\}_{n \geqslant 0}$ such that $\lambda_n \xrightarrow[n \to \infty]{\mathcal{R}} 0$. The random perturbation P_n in (3) is taken as

$$P_n = \lambda_n Z_n . \tag{9}$$

Thus, (3) generates a sequence of random vectors $\{X_n\}_{n \geqslant 0}$ such that, for $n \geqslant 0$:

$$X_{n+1} = Q(X_n) + \lambda_n Z_n . \tag{10}$$

We assume that Z_n is a random vector (R.V.) such that

$$\forall n \geqslant 0: Z_n \in B \text{ almost surely (a.s.)}, \tag{11.1}$$

i.e., $P(Z_n \in B) = 1$, for all $n \geqslant 0$;

$$\forall n \geq 0\text{: } Z_n \text{ is independent of } X_i\,, \quad i = 0, \ldots, n\,. \tag{11.2}$$

We take $Z_n = Z$, independent of n, where Z is defined as follows: let χ_B be the indicator function of B and

$$|B| = \int_B \exp\left(-\frac{1}{2}|x|^2\right) dx\,.$$

Z is an N-dimensional R.V. having the distribution defined by the density function

$$f(x) = \frac{\chi_B(x)}{|B|} \exp\left(-\frac{1}{2}|x|^2\right), \quad \forall x \in E\,. \tag{12}$$

The conditional distribution function of X_{n+1} is (see also Appendix A1)

$$F_{n+1}(y \mid X_n = x) = F\left(\frac{y - Q(x)}{\lambda_n}\right).$$

The associated density function f_{n+1} is

$$f_{n+1}(y \mid X_n = x) = \frac{1}{\lambda_n^N} f\left(\frac{y - Q(x)}{\lambda_n}\right). \tag{13}$$

Until the end of Section 4, the construction (12), (13) will be used. Other methods of generation are considered in Section 5 meanwhile.

Let us explain already the selection of parameter λ_n which implies the boundness and convergence results in Sections 3 and 4. We consider a parameter $\varepsilon > 0$, small enough, and we set

$$\lambda_n = \sqrt{\frac{c}{\log(n+d)}}\,. \tag{14}$$

If

$$c > \frac{1}{2}\beta^2\,; \quad d > \exp(c/(1 - \sqrt{1-\varepsilon})^2) \tag{15}$$

then (see Appendix A2, 2)

$$\forall n \geq 0\text{: } 0 < \lambda_n < 1 - \sqrt{1-\varepsilon}\,. \tag{16}$$

This inequality is used in the proof of the enounced theorems.

3. Boundness of the R.V. Sequence

In this section it is established that the sequence of R.V. $\{X_n\}_{n\geq 0}$ generated by the algorithm (10) from the initial guess $X_0 \in E$ is bounded for suitable μ: convergence results are inferred in Section 4. We set $\alpha = \alpha(R)$, $a = a(R)$, B_ε the ball $\sqrt{1-\varepsilon}B$:

$$B_\varepsilon = \{x \in E \,|\, |x| \leq R\sqrt{1-\varepsilon}\}\,.$$

We consider strictly positive real numbers R and ε such that

$$0 < \varepsilon < \frac{\alpha^2}{a^2}, \quad R\sqrt{1-\varepsilon} > R_c + 2\,. \tag{17}$$

Since $\alpha/a \leq 1/R$,

$$\frac{\alpha}{a^2}\left[1 + \sqrt{1 - \frac{a^2\varepsilon}{\alpha^2}}\right] < 2\frac{\alpha}{a^2} \leq \frac{2}{aR} \leq \frac{R\sqrt{1-\varepsilon} - R_c}{aR}\,. \tag{18}$$

PROPOSITION 3.1. *Let* μ *be such that*

$$\frac{\alpha}{a^2}\left[1 - \sqrt{1 - \frac{a^2\varepsilon}{\alpha^2}}\right] < \mu < \frac{\alpha}{a^2}\left[1 + \sqrt{1 - \frac{a^2\varepsilon}{\alpha^2}}\right]. \tag{19}$$

Then $Q(B) \subset B_\varepsilon$.

REMARK. The condition (19) is *implicit*: it does not define explicit bounds for μ, since the calculation of the ratio α/a^2 leads to a new problem of optimization, which may be more complicated than the one corresponding to the minimization of J itself. Nevertheless, we can obtain explicit bounds for μ, under the conditions below, relevant from the practical stand point. It can be assumed: there exists $\eta > 0$ such that

$$|x| \geq R_c \Rightarrow (\nabla J(x), x) \geq \eta |x|^2\,.$$
$$\exists \{M_1, M_2\} \subset \mathcal{R}^+ \colon M_1 \leq \sup_B |\nabla J(x)| \leq M_2\,.$$

In this case, (4.2) holds with $\alpha(R) \geq \eta$. Further ratio α/a^2 remains within the interval $[\eta R_c^2/M_2, M_2 R/M_1^2]$, as it is shown by a simple calculation. This condition gives us explicit bounds to deal with condition (19).

Proof of Proposition 3.1.

1. The condition (19) implies that

$$\varepsilon - 2\mu\alpha + \mu^2 a^2 \leq 0\,.$$

Let $x \in B$ be given such that $R_c \leq |x| \leq R$. (2), (4.2) and (4.3) imply the estimate

$$|Q(x)|^2 \leq R^2 - 2\mu\alpha R^2 + \mu^2 a^2 R^2\,.$$

Thus,

$$|Q(x)|^2 \leq (1-\varepsilon)R^2\,, \quad \text{if } R_c \leq |x| \leq R\,.$$

2. Let $x \in B$ be given such that $|x| \leq R_c$. Since (see (18))

$$0 < \mu < \frac{R\sqrt{1-\varepsilon} - R_c}{aR}, \tag{20}$$

(2) and (4.3) yield the estimate

$$|Q(x)| \leq R_c + \mu aR \leq R\sqrt{1-\varepsilon}\,.$$

3. The proposition follows from 1 and 2.

THEOREM 3.2. *Let* μ *satisfy* (19) *and* λ_n *verify* (16). *If*

$$X_0 \in B \text{ a.s.} \tag{21}$$

then

$$\{X_n\}_{n\geq 0} \subset B \text{ a.s.},$$

that is to say the sequence remains in B almost surely.

Proof.

1. We denote by B_n the event "$|P_n| \leq (1-\sqrt{1-\varepsilon})R$". It follows from (11.1) and (16) that

$$\forall n \geq 0\colon P(B_n) = 1\,. \tag{22}$$

2. We note E_n the event "$X_n \in B$". The aim is to prove that

$$P(E) = 1,\ E = \bigcap_{n=0}^{+\infty} E_n\,.$$

Let E_n^c be the complement of E_n (the event "$X_n \notin B$") and E^c be the complement of E. We have, from the basic properties of probabilities (see, for instance [4]).

$$P(E^c) = P\left(\bigcup_{n=0}^{+\infty} E_n^c\right) \leq \sum_{n=0}^{+\infty} P(E_n^c)\,.$$

Thus, we have only to show that

$$\forall n \geq 0\colon P(E_n^c) = 0\,, \tag{23}$$

which will imply $P(E^c) = 0$, or equivalently $P(E) = 1$.

3. The proof of (23) is carried out by induction:
   a. We have $P(E_0) = 1$ (hypothesis (21) of the theorem).
   b. Let us suppose that $P(E_n) = 1$. We denote by A_n the event "$Q(X_n) \in B_\varepsilon$". It follows from the Proposition 3.1 that

$$E_n \subset A_n \Rightarrow P(A_n) \geq P(E_n \cap A_n) = P(E_n) = 1\,. \tag{24}$$

   c. It follows from the estimate

$$|X_{n+1}| \leq |Q(X_n)| + |P_n|$$

that

$$A_n \cap B_n \subset E_{n+1} \Rightarrow P(E_{n+1}) \geq P(A_n \cap B_n) .$$

But, from (22), (24):

$$P(A_n \cap B_n) = 1$$

and we have $P(E_{n+1}) = 1$.

4. Convergence to a Global Minimum

Let us introduce

$$U_n = \min\{J(X_i): 0 \leq i \leq n\} . \tag{25}$$

$\{U_n\}_{n \geq 0}$ is a monotonous decreasing and bounded from below by $m = m(R)$. Thus,

$$\exists U \geq m: U_n \xrightarrow[n \to \infty]{} U . \tag{26}$$

We have the following result:

PROPOSITION 4.1. *If there exists* $\delta > 0$ *such that, for all* $\theta \in]m, m + \delta[$ *the following conditions are satisfied*:

$$P(U_{n+1} < \theta \mid U_n \geq \theta) \geq c(\theta, n) > 0 \tag{27.1}$$

and

$$\sum_{n=0}^{+\infty} c(\theta, n) = +\infty \tag{27.2}$$

then

$$U = m \ a.s.$$

Proof. The proof is carried out by using arguments analogous to those of [10], [11]:

1. Let $\theta \in]m, m + \delta[$. We set $p_n = P(U_n < \theta)$. We shall establish that

$$p_n \xrightarrow[n \to \infty]{\mathscr{R}} 1 . \tag{28}$$

a. Since $\{U_n\}_{n \geq 0}$ is monotonous decreasing, we have

$$U_n < \theta \Rightarrow U_{n+1} < \theta$$

and it is derived

$$\forall n \geq 0: 1 \geq p_{n+1} \geq p_n \geq 0 , \tag{29}$$

equivalently, the sequence $\{p_n\}_{n \geq 0}$ is monotonous increasing. Thus, there exists $p \in \mathscr{R}$ such that

$$0 \leq p \leq 1; \ p_n \xrightarrow[n \to \infty]{\mathscr{R}} p . \tag{30}$$

b. Let us suppose that

$$p < 1 . \tag{31}$$

We have

$$p_{n+1} = P(U_{n+1} < \theta, U_n < \theta) + P(U_{n+1} < \theta, U_n \geq \theta) . \tag{32}$$

But, on the one hand,

$$P(U_{n+1} < \theta, U_n < \theta) = P(U_n < \theta) = p_n ,$$

since the sequence $\{U_n\}_{n \geq 0}$ is decreasing, on the other hand,

$$\begin{aligned} P(U_{n+1} < \theta, U_n \geq \theta) &= P(U_n \geq \theta).P(U_{n+1} < \theta \mid U_n \geq \theta) \\ &\geq (1 - p_n)c(\theta, n) . \end{aligned}$$

That way, it follows from (29), (30) and (32) that

$$p_{n+1} \geq p_n + (1 - p_n)c(\theta, n) \geq p_n + (1 - p)c(\theta, n) . \tag{33}$$

By adding inequalities (33) for $n = 0, \ldots, i$, we obtain

$$p_{i+1} \geq p_0 + (1 - p) \sum_{n=0}^{i} c(\theta, n)$$

and (27.2) implies that $p_n \xrightarrow[n \to \infty]{\mathcal{R}} + \infty$, what is in contradiction with (30). Thus, (31) does not hold and we have $p = 1$.

2. Let $k_0 = \min\{k \in \mathcal{N} - \{0\} \mid \delta \leq 1/k\}$. For $k \geq k_0$, E_k is the event "$U \geq m + 1/k$" and we set $q_k = P(E_k)$. We have $q_k = 0$, since, by choosing $\theta \in]m + 1/k, m + \delta[$, we obtain

$$U \geq \theta \Rightarrow U_n \geq \theta , \quad \forall n \geq 0 ,$$

what implies that

$$\forall n \geq 0 \colon 0 \leq q_k \leq P(U_n \geq \theta) = 1 - p_n \xrightarrow[n \to \infty]{\mathcal{R}} 0 .$$

But

$$P(U > m) = P\left(\bigcup_{k=k_0}^{+\infty} E_k \right) \leq \sum_{k=k_0}^{+\infty} P(E_k) = 0$$

and we have $P(U = m) = 1$.

We have the following convergence result

THEOREM 4.2. *Suppose that $Z_n = Z$, for all $n \geq 0$, where the distribution of Z is defined by* (12), *and λ_n is given by* (14), *with parameters c, d verifying* (15). *If $X_0 \in B$, then*

$$U = m \ a.s.$$

Proof (supplemental lines are moved to Appendix A2).

1. Let S_θ be defined by (4.5). From (11.2), the relation (10) defines a Markov Chain such that

$$P(X_{n+1} \in S_\theta \mid X_i \not\in S_\theta, i = 0, \ldots, n) = P(X_{n+1} \in S_\theta \mid X_n \not\in S_\theta) . \tag{34}$$

2. The second inequality in (15) implies that (16) is satisfied: thus $X_n \in B$ a.s. and, from (34) (see for instance [4]),

$$P(X_{n+1} \in S_\theta, X_n \not\in S_\theta) = \int_{B - S_\theta} P(X_n \in dx) \int_{S_\theta} f_{n+1}(y \mid X_n = x)\, dy .$$

3. This result and the definition of the conditional probability,

$$P(X_{n+1} \in S_\theta \mid X_n \not\in S_\theta) = P(X_{n+1} \in S_\theta, X_n \not\in S_\theta)/P(X_n \not\in S_\theta) ,$$

yield the estimate

$$P(X_{n+1} \in S_\theta \mid X_n \not\in S_\theta) \geq \inf_{x \in B - S_\theta} \left\{ \int_{S_\theta} f_{n+1}(y \mid X_n = x)\, dy \right\} .$$

4. We have

$$P(U_{n+1} < \theta \mid U_n \geq \theta) = P(X_{n+1} \in S_\theta \mid X_n \not\in S_\theta) . \tag{35}$$

Thus, from (8), (12), (13), (35),

$$P(U_{n+1} < \theta \mid U_n \geq \theta) \geq c(\theta, n) = \gamma(\theta) \exp\left(- \frac{[\beta(R)]^2}{2\lambda_n^2} \right) \Big/ \lambda_n^N , \tag{36}$$

where

$$\gamma(\theta) = \frac{1}{|B|} \operatorname{meas}(S_\theta) .$$

5. From (4.6), we have that: there exists $\delta > 0$ such that

$$\forall \theta \in]m, m + \delta[: c(\theta, n) > 0$$

and condition (27.1) is satisfied.

6. Moreover, (14) implies that

$$c(\theta, n) = \gamma(\theta) \frac{[\log(n + d)]^{N/2}}{c^{N/2}(n + d)^{[\beta(R)]^2/2c}}$$

and, from (36) and the first inequality in (15), we have

$$\sum_{n=0}^{+\infty} c(\theta, n) = +\infty .$$

So, condition (27.2) is satisfied.

7. The result follows from Proposition 4.1.

5. Numerical Experiments

The arguments developed in Section 2.2 suggest the following numerical algorithm:

STEP 0 Select $x_0 \in B$.

STEP $n+1$ $(n \geq 0)$

1 Generate k values from Z defined by density (12), by a simulation procedure. The values generated are denoted by $Z_1, \ldots, Z_k$.

2 Set $Z_0 = 0$ and
$X_{n+1} = \text{Arg Min}\{J(Q(X_n) + \lambda_n Z_i)\colon 0 \leq i \leq k\}$.

This method furnishes a sequence $\{X_n\}_{n \geq 0} \subset B$ provided (14), (15) and (19) are satisfied. If U_n is defined by (25), we have

$$U_n \xrightarrow[n \to \infty]{\mathcal{R}} m \quad \text{(a.s.)}.$$

In practice, the iterations are stopped when $n = nmax$ and we approximate $m \approx U_{nmax}$.

5.1. METHOD M1

The main difficulty in the implementation of this algorithm is the simulation of the random vector Z with density (12): the use of discrete markovian approximation methods as those of [2] can be expansive in CPU time. In order to obtain faster calculations, the generation of a value $Z_i = ((Z_i)_1, \ldots, (Z_i)_N)$ from Z is performed as follows:

a. Generate a value Y from the standard deviate N-dimensional Gaussian distribution $\mathcal{N}(0, Id)$.

b. *If* $Y \in B$, *then* set $Z_i = Y$ *else* generate a value U from the uniform deviate distribution on $(0, 1)$ and set $Z_i = U.Y/R$.

In the sequel, this method is referred to as being the method M1.

5.2. METHOD M2

Several authors have considered a different situation, where B *is not* a ball *but*

$$B = \prod_{j=1}^{N} [XMIN_j, XMAX_j]. \tag{37}$$

Results about the asymptotic behaviour of the diffusion

$$dXt = -\nabla J(X_t)dt + \lambda_t dZ_t \tag{38}$$

show that $\lim_{t\to+\infty} J(X_t) = m$ a.s. (see for instance [7]).

When B is defined by (37), (10) can be interpreted as a discretization of (38). In this case, the generation of a value Z_i from Z can be performed as follows:

a. Generate a value Y from the standard deviate N-dimensional Gaussian distribution $\mathcal{N}(0, Id)$.

b. Let us introduce $h_j = XMAX_j - XMIN_j > 0$. Let us denote the $\mathcal{Z}$ the set of relative integers. There is an integer $n_j \in \mathcal{Z}$ such that $XMIN_j \leqslant Y_j - n_j h_j \leqslant XMAX_j$. We set $(Z_i)_j = Y_j - n_j h_j$.

This method is denoted by $M2$.

5.3. METHOD M3 AND GENERALITIES ABOUT THE NUMERICAL TESTS

The results obtained by M1 and M2 are compared to the deterministic gradient method, denoted by M3, where the values X_n are generated by (1)–(2). This comparison gives us information about the effect of the random perturbation.

In practice, the conditions of Theorem 4.2 may be pessimistic, nevertheless we can obtain convergence even if c and d do not satisfy (15): all the performed experiments use

$$\lambda_n = \sqrt{\frac{c}{\log(n+1)}}, \text{ i.e., } d = 1 .$$

The initial guess is $X_0 = 0$ and the values Y from the standard deviate gaussian distribution $\mathcal{N}(0, Id)$ are obtained by the usual log-trigonometric generator (see, for instance [10]).

5.4. APPROXIMATION BY A SUM OF EXPONENTIALS

In this example. $N = 2NEXP$ and

$$J(x) = \frac{1}{41} \sum_{j=1}^{41} \left[y_j - \sum_{i=1}^{NEXP} x_{2i-1} \exp(x_{2i} t_j) \right]^2 ,$$

where, for $j = 1, \ldots, 41$,

$$t_j = (j-1)/40; \; y_j = 1 + \log(1 + t_j) .$$

This can be interpreted as the least squares fitting of a sum of $NEXP$ exponentials to discrete data given by (t_j, y_j), $j = 1, \ldots, 41$. The goodness of the fit is controlled by $E = \sqrt{J(x)}$ and the relative errors

$$ER_{max} = \max_{1 \leqslant j \leqslant 41} \left| y_j - \sum_{i=1}^{NEXP} x_{2i-1} \exp(x_{2i} t_j) \right| \Big/ |y_j| ;$$

$$ER_2 = E \Big/ \left(\frac{1}{41} \sum_{j=1}^{41} y_j^2 \right)^{1/2} .$$

E gives the absolute error in the mean square norm, $ER_{\max}$ and ER_2 provide pointwise and global control of the quality of the final fit, respectively.

5.4.1. *An example with variable NEXP*

We consider five values of NEXP: 1, 2, 3, 4 and 5. The methods run with the following sets of parameters:

$$\mu = 0.125\,, \quad k = 5000\,, \quad nmax = 250\,, \quad R = 2.5 \quad NEXP\,, \quad c = 1\,,$$

$$XMIN_j = \begin{cases} -5\,, & \text{if } j \text{ is even}\,; \\ -\infty\,, & \text{if } j \text{ is odd}\,, \end{cases} \qquad XMAX_j = \begin{cases} 5\,, & \text{if } j \text{ is even}\,; \\ +\infty\,, & \text{if } j \text{ is odd}\,. \end{cases}$$

The results obtained are shown in Table I: in this situation, the behaviour of M1 and M2 is analogous. The two methods converge to points which are very close and the value of J is reduced into a significant way. The behaviour of M3 is bad when compared to the other methods: errors furnished by M3 are about 100 times greater than errors furnished by M1 and M2. Experiments performed with these two methods, using different values $\mu \in [0.1, 0.5]$ have led to results analogous to Table I. (The behaviour of M3 is worse for increasing μ.)

5.4.2. *An example with fixed NEXP*

In this example, we choose $NEXP = 5$, $\mu = 0.25$, $R = 12.5$. Other parameters have the same value as in 5.4.1. The results obtained are shown in Table II.

The evolution of E is in Figure 1: we observe that the random perturbation has a significant effect on the convergence.

Table I. Results for $\mu = 0.125$

NEXP	1	2	3	4	5
E	$3E-2$	$1E-2$	$2E-4$	$6E-4$	$8E-4$
ER_{max}	8%	3%	0.08%	0.1%	0.1%
ER_2	2%	0.7%	0.02%	0.04%	0.06%

(a) Results of M1.

NEXP	1	2	3	4	5
E	$3E-2$	$1E-2$	$2E-4$	$6E-4$	$7E-4$
ER_{max}	8%	3%	0.08%	0.1%	0.1%
ER_2	2%	0.7%	0.02%	0.04%	0.05%

(b) Results of M2.

NEXP	1	2	3	4	5
E	$3E-2$	$3E-2$	$3E-2$	$3E-2$	$4E-2$
ER_{max}	8%	8%	9%	10%	11%
ER_2	2%	2%	2%	2%	3%

(c) Results of M3.

Table II. Results for $NEXP = 5$ ($\mu = 0.25$)

	E	ER_{max}	ER_2
$M1$	$9E-4$	0.2%	0.06%
$M2$	$4E-4$	0.05%	0.03%
$M3$	0.16	35%	12%

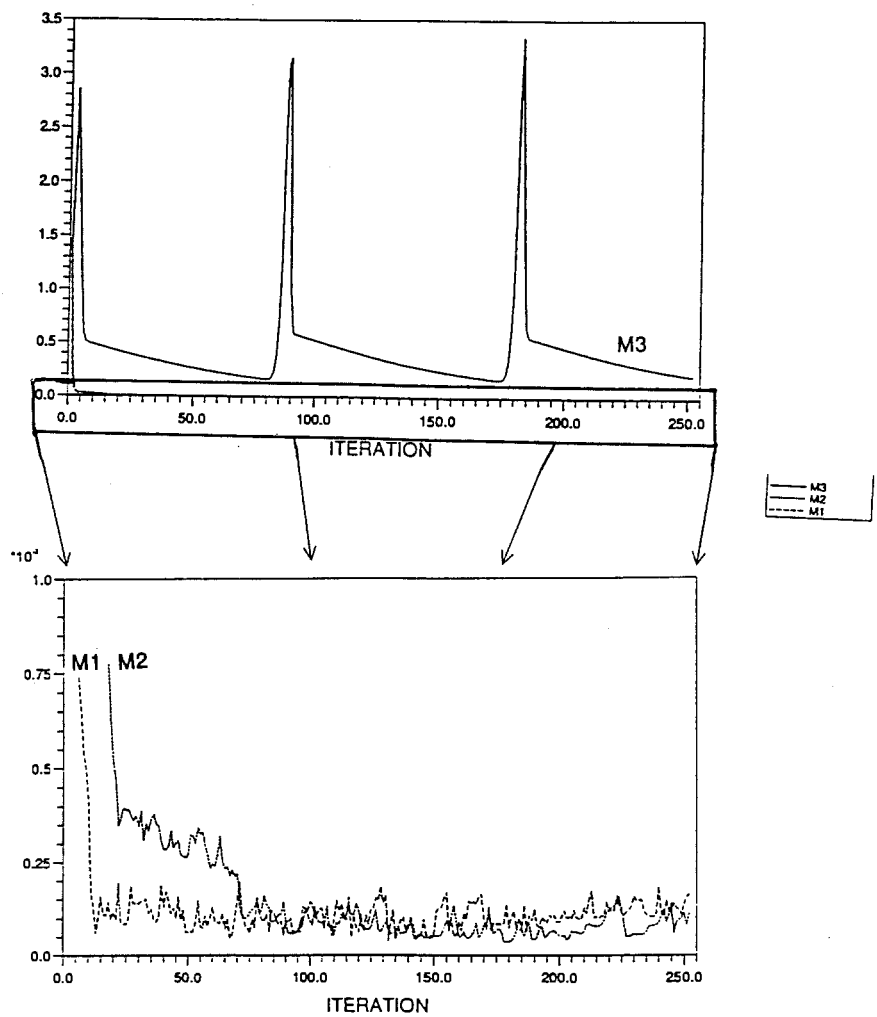

Fig. 1. Evolution of E.

The curves obtained are shown in Figure 2: the results of M1 and M2 are very close on the interval [0, 1.0], where the data is given. However, if the calculated solutions are extrapolated on [1.0, 2.5], the results of M1 are not so good, while those of M2 remain very close to the exact curve. If the quality of the approximation is measured by quantities E, ER_{max}, ER_2 analogous to those

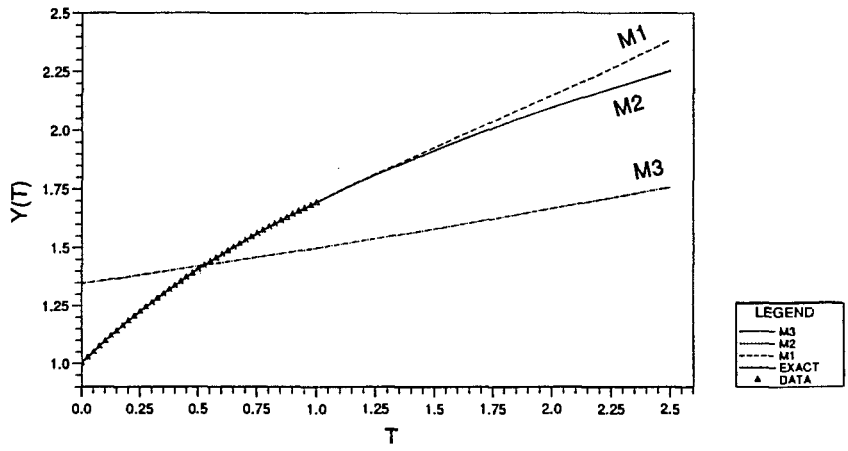

Fig. 2. Curves obtained.

previously defined but involving (t_j, y_j), $j = 1, \ldots, 101$ (instead of $j = 1, \ldots, 41$), we have the results as shown in Table III.

5.4.3. *Influence of k*

In this example, all the parameters are set to the values of 5.4.2, except k, which is variable. We use $M1$ with $k = 0$, 100, 2000, 5000, 10000. The value $k = 0$ corresponds to $M3$ and the results are in Table IV.

This behaviour is quite intuitive: the greater is k, the better the distribution of Z is simulated and more information is obtained about the minima of J. The evolution of E is shown in Figure 3: we observe that

Table III. Errors in the extrapolation

	E	ER_{max}	ER_2
$M1$	$8E-2$	7%	3%
$M2$	$3E-3$	0.15%	0.1%
$M3$	0.5	35%	18%

Table IV. Influence of k

k	0($M3$)	100	2000	5000	10000
E	0.16	$6E-3$	$2E-3$	$9E-4$	$8E-5$
ER_{max}	35%	0.9%	0.3%	0.2%	0.02%
ER_2	12%	0.4%	0.2%	0.06%	0.006%

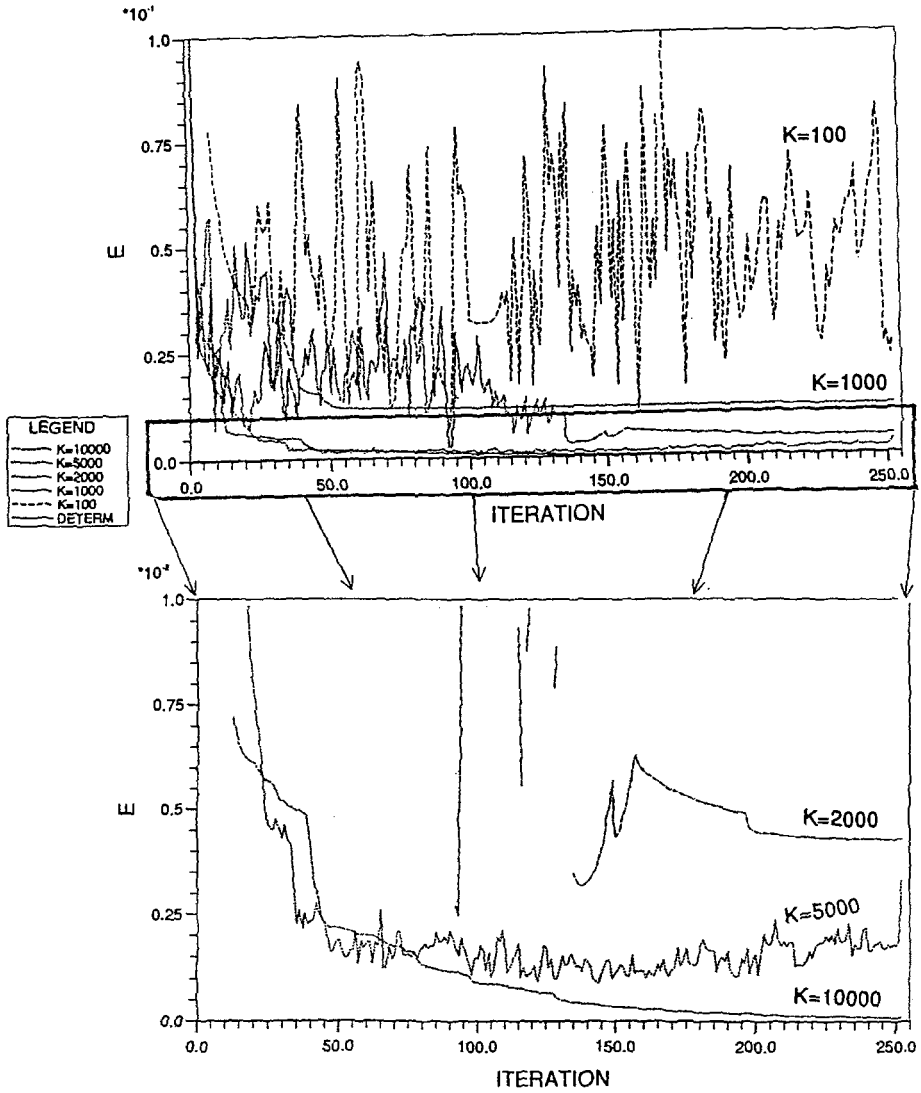

Fig. 3. Evolution of E.

- on the one hand, even with $k = 100$, the effect of the random perturbation is significant and E is reduced when compared to M3;
- on the other hand, the rule of the random perturbation in the reduction of E increases with the iterations: for small n, the behaviour is analogous for all the values of k. However, the smaller is k, the faster is the stabilisation of the method: we observe also that E decreases until $n = n(k)$ and becomes oscillating for $n > n(k)$, where $n(k)$ increases with k. This behaviour suggests

that the method can be possibly improved by using a variable k instead of a fixed number of simulations: $k = k(n)$, increasing with n.

5.5. SOLUTION OF A LARGE SYSTEM OF NONLINEAR EQUATIONS

In this example, $N = 4950$. We consider the following Boundary Value Problem (B.V.P.) for the unknown function φ and given cosntants $K > 0$ and $l > 0$:

$$\begin{cases} \partial_1(a(\partial_1\varphi)\partial_1\varphi) + \partial_2^2\varphi = 0 & \text{in} \quad \Omega\,, \\ \varphi = 0 & \text{on} \quad \Gamma'\,, \\ \partial_2\varphi = g & \text{on} \quad \Gamma\,. \end{cases} \tag{39}$$

The partial derivatives with respect to the variables x_1 and x_2 are denoted by ∂_1 and ∂_2 respectively and we choose

$$\Omega =]0, 2[\times]0, 1[\subset \mathcal{R}^2; \quad \partial\Omega = \text{boundary of } \Omega \tag{40.1}$$

$$\Gamma = \{(x_1, x_2) \in \partial\Omega; \quad x_2 = 0\}; \quad \Gamma' = \partial\Omega - \Gamma; \tag{40.2}$$

$$\begin{cases} a(s) = K - ls; & K = 6.25\left(\dfrac{1}{M} - M\right); \quad l = 1.2\,, \\ g(x_1) = \begin{cases} \sqrt{M}(-4x_1)\,, & x_1 \in (\frac{1}{2}, \frac{3}{2})\,, \\ 0, & \text{otherwise}\,. \end{cases} \end{cases} \tag{40.3}$$

The first equation in (39) is of mixed type elliptic/hyperbolic, what means a difficulty for significant data as (40.3). When this B.V.P. is approximated by a Finite Element Method, a grid made of $1 + N1$ vertical and $1 + N2$ horizontal straight lines is introduced. Let us set $h_1 = 2/N1$ and $h_2 = 1/N2$: function φ is approximated by the value φ_{ij} at the point $P_{ij} = ((i-1)h_1, (j-1)h_2)$ and the set of unknowns is $\Phi = (\varphi_{ij})$; $i = 2, \ldots, N1$; $j = 1, \ldots, N2$. The number of unknowns is $N2(N1 - 1)$ and Φ satisfies a nonlinear system:

$$E_{ij}(\Phi) = 0, \quad i = 2, \ldots, N1, \quad j = 1, \ldots, N2\,,$$

where (see [9] for details)

$$\begin{aligned} &\text{for } j = 1: \\ &E_{ij}(\Phi) = c_2 a_{ij}(-\varphi_{i-1j} + 2\varphi_{ij} - \varphi_{i+1j}) \\ &\qquad - 2c_1(\varphi_{ij} - \varphi_{ij+1}) - s_i\,, \\ &\text{for } j = 2, \ldots, N2: \\ &E_{ij}(\Phi) = c_2 a_{ij}(-\varphi_{i-1j} + 2\varphi_{ij} - \varphi_{i+1j}) \\ &\qquad - c_1(-\varphi_{ij-1} + 2\varphi_{ij} - \varphi_{ij+1})\,. \end{aligned}$$

Here we have set

$$\begin{cases} c_1 = -h_1/h_2\,, \quad c_2 = -h_2/h_1\,, \quad s_i = -2h_1 g((i-1)h_2)\,, \\ \qquad\qquad a_{ij} = K - l(\varphi_{i+1j} - \varphi_{i-1_j})/h_1\,. \end{cases}$$

In [9], this problem has been solved by the following Deterministic Iterative Method (DIM):

STEP 0 Select an initial guess Φ^0.

STEP $n+1$ $(n \geqslant 0)$

For $i := 2$ **step** 1 **until** $N1$ **do**
  For $j := 1$ **step** 1 **until** $N2$ **do**
    $\phi_{ij} := \phi_{ij} - \mu E_{ij}(\Phi)$;
  end ;
end .

This method is analogous to a gradient method with a fixed parameter and we shall analyze its behaviour under random perturbations: let us introduce a Random Perturbation Method (RPM) where step $n+1$ is performed as follows:

STEP $n+1$ $(n \geqslant 0)$
For $i := 2$ **step** 1 **until** $N1$ **do**
  For $j := 1$ **step** 1 **until** $N2$ **do**
    (i) Generate k values from $\mathcal{N}(0, 1)$,
    the standard deviate gaussian distribution.
    The values generated are denoted by $Z_1, \ldots, Z_k$.
    (ii) Set $Z_0 = 0$ and $\varphi_{ij} = \psi_{ij}^{opt} = (\Psi)_{ij}$,
    $\Psi^{opt} = \text{Arg Min}\{|E_{ij}(\Psi^p)|\colon 0 \leqslant p \leqslant k\}$
    $\Psi^p = (\psi_{ij}^p)$
    $\psi_{ij}^p = \varphi_{ij} - \mu E_{ij}(\Phi) - \lambda_n Z_p$,
    $\psi_{rs}^p = \phi_{rs}, r \neq i$ or $s \neq j$.
  end ;
end .

The quality of the approximated solution Φ^n is controlled by the mean value and the local residue given respectively by:

$$RM = \left(h_1 h_2 \sum_{i=2}^{N_1} \sum_{j=1}^{N_2} |E_{ij}(\Phi^n)|^2\right)^{1/2}, \tag{41}$$

$$RL = Max\left\{\frac{1}{h_1} |E_{ij}(\Phi^n)|\colon i = 2, \ldots, N1,\ j = 1, \ldots, N_2\right\}. \tag{42}$$

In the experiments, $M = 0.9$ and the FEM involves a grid with $N1 = 100$,

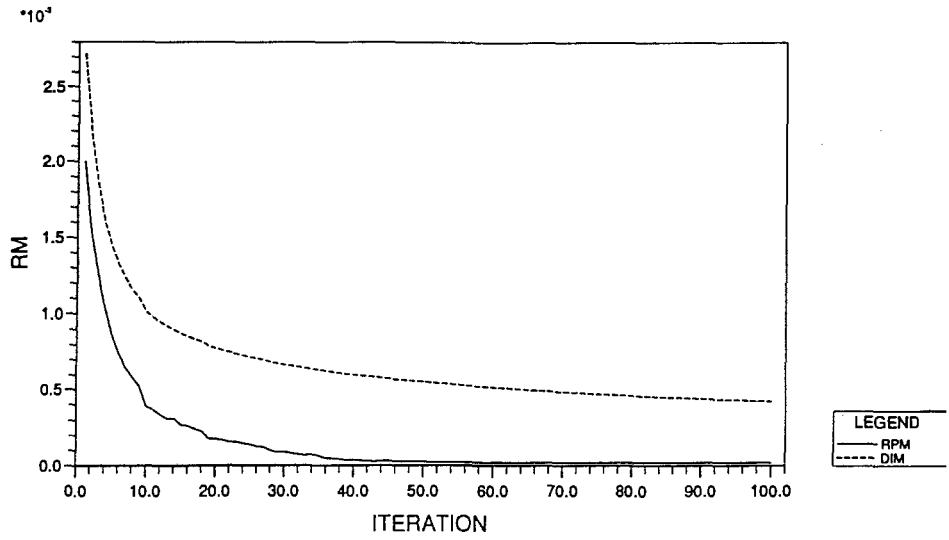

Fig. 4. Evolution of *RM*.

$N2 = 50$. In this case, the number of unknowns is 4950. The results are shown in Figures 4 and 5 and in Tables V and VI. The selected parameters are $\mu = 0.1$, $k = 100$, $nmax = 100$, $c = 1.0\ E - 6$. The initial guess is $\Phi^0 = 0$.

As we observe in Tables V and VI and Figures 4 and 5, both the values of *RM* and *RL* are weakened by the random perturbation: the final values furnished by RPM are about 50 times smaller than the values obtained by *DIM*. In fact, these values are 10 times smaller than the values furnished by *DIM* after 500 iterations:

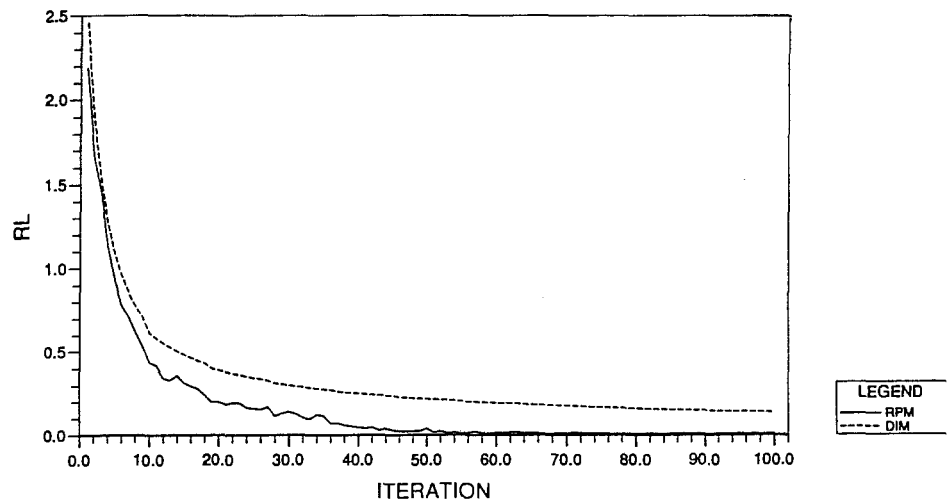

Fig. 5. Evolution of *RL*.

Table V. Evolution of *RM*

n	1	25	50	75	100
DIM	2.7E − 3	7.2E − 4	5.5E − 4	4.7E − 4	4.2E − 4
RPM	2.0E − 3	1.3E − 4	2.6E − 5	2.0E − 5	2.0E − 5

Table VI. Evolution of *RL*

n	1	25	50	75	100
DIM	2.5E + 0	3.4E − 1	2.2E − 1	1.7E − 1	1.4E − 1
RPM	3E − 1	1.6E − 1	4.0E − 2	1.1E − 2	8.8E − 3

the random perturbation has a non negligible effect. Moreover, after 100 iterations hyperbolic zones occur only in the *RPM*. For the approximated solution calculated by *DIM*, the whole Ω is an elliptic zone and no change of type occurs: the occurrence of hyperbolic zones in *DIM* needs about 300 iterations.

6. Concluding Remarks

The gradient method with a fixed parameter can be interpreted as a relaxation procedure for the system of nonlinear equations $\nabla J(x) = 0$. So, it can fail to find global minima of J. The results stated in Sections 3 and 4 show that suitable random perturbations of this method avoid convergence to local minima and yield almost sure convergence to a global minimum. Further the difficult choice of an initial guess in order to neighbour the global minimum of J does not occur.

These results suggest a modification of the gradient method and lead to an algorithm: its implementation is easy and its numerical behaviour has been tested in Section 5 for the least squares fitting of a sum of exponentials and a nonlinear system for a great number of unknowns. The effect of the random perturbation has been examined by comparison with the usual deterministic gradient method: for the considered examples, this effect is not negligible and significantly better results are obtained when a random perturbation is introduced. Namely when reducing the residues associated with the approximated quantities, it is observed that the gradient method with a random perturbation leads to decreasing residues as the number of iterates increases. It is not the same when using the gradient method without a random perturbation: actually the residues are not reduced or oscillate as soon as a number of iterates is performed.

The study of gradient methods with a variable parameter (μ_n instead of μ in (2)) has not been performed here. This modification is connected to the Robbins–Monro algorithm (see, for instance [4]) and can be useful for the situations where the cost function can be only approximated and not exactly evaluated and would induce probably attractive investigations.

Appendix

A1. SUPPLEMENTAL LINES FOR THE CONSTRUCTION (12), (13)

Since we choose $Z_n = Z$, the equality below holds (from (10))

$$(X_{n+1} < y, X_n = x) = \left(Z < \frac{y - Q(x)}{\lambda_n}, X_n = x\right).$$

From (7.2), one has

$$P(X_{n+1} < y \mid X_n = x) = P\left(Z < \frac{y - Q(x)}{\lambda_n} \,\middle|\, X_n = x\right),$$

that is to say, the conditional distribution function of X_{n+1} is given by

$$F_{n+1}(y \mid X_n = x) = F\left(\frac{y - Q(x)}{\lambda_n}\right).$$

A2. SUPPLEMENTAL LINES FOR THE PROOF OF THEOREM 4.2

1. By the same arguments as those in A1, (10) and (11.2) imply that when the values of X_i, $i = 0, \ldots, n$ are given, the conditional probability of X_{n+1} reduces to the one where only the value of X_n is given. That is to say, relation (10) defines a Markov chain so that (34) holds.
2. We have $\lambda_n > 0$, since $c > 0$, $n \geq 0$, $d > 1$. Moreover, the second inequality in (15) implies that

   $$n + d > \exp(c/(1 - \sqrt{1 - \varepsilon})^2).$$

   So,

   $$\log(n + d) \geq c/(1 - \sqrt{1 - \varepsilon})^2$$

   and (16) holds. Thus, from Theorem 3.2, $X_n \in B$ a.s., so that

   $$(X_{n+1} \in S_\theta, X_n \notin S_\theta) = (X_{n+1} \in S_\theta, X_n \in B - S_\theta).$$

   A classical result on conditional distributions (see [4] for instance) implies that

   $$P(X_{n+1} \in S_\theta, X_n \notin S_\theta) = \int_{B - S_\theta} P(X_n \in \mathrm{d}x) \int_{S_\theta} f_{n+1}(y \mid X_n = x)\, \mathrm{d}y.$$

3. From 2, it is inferred that

   $$P(X_{n+1} \in S_\theta, X_n \notin S_\theta) \geq P(X_n \notin S_\theta) \inf_{x \in B - S_\theta} \left\{ \int_{S_\theta} f_{n+1}(y \mid X_n = x)\, \mathrm{d}y \right\}.$$

4. From (25), one has

   $$(U_n \geq \theta) = (J(X_i) \geq \theta,\ i = 0, \ldots, n).$$

   and

$$(U_{n+1} < \theta, U_n \geq \theta) = (J(X_{n+1}) < \theta, (J(X_i) \geq \theta, i = 0, \ldots, n)).$$

From (4.5), it follows that

$$(U_n \geq \theta) = (X_i \notin S_\theta, i = 0, \ldots, n)$$

and

$$(U_{n+1} < \theta, U_n \geq \theta) = (X_{n+1} \in S_\theta, (X_i \notin S_\theta, i = 0, \ldots, n)).$$

The definition of the conditional probability implies that

$$P(U_{n+1} < \theta \mid U_n \geq \theta) = P(X_{n+1} \in S_\theta \mid (X_i \notin S_\theta, i = 0, \ldots, n))$$

and 1 yields (35). This and 3 yield

$$P(U_{n+1} < \theta \mid U_n \geq \theta) \geq \inf_{x \in B - S_\theta} \left\{ \int_{S_\theta} f_{n+1}(y \mid X_n = x)\, dy \right\}.$$

Coming back to (8) and (13), elementary boundedness arguments lead to (36).

5. The assertions are obvious.
6. A simple calculation furnishes the expression of $c(\theta, n)$ in terms of γ, β, c, d. The first inequality in (15) implies that

$$\frac{\beta^2}{2c} < 1 \underset{n \geq 0, d > 1}{\Rightarrow} \frac{1}{n+d} \leq \frac{1}{(n+d)^{[\beta(R)]^2/2c}}$$

and we obtain the estimate

$$c(\theta, n) \geq \frac{\gamma(\theta)}{c^{N/2}} \frac{[\log(n+d)]^{N/2}}{n+d},$$

which makes series $\Sigma_n\, c(\theta, n)$ divergent, that is, (27.2).

7. The results in 4 and 6 imply that assumptions (27.1) and (27.2) are satisfied. Thus, sequence $\{U_n\}_{n \geq 0}$ converges almost surely towards $U = m$ (Proposition 4.1).

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