Numer. Math. 70: 119–128 (1995)

Numerische
Mathematik

Error analysis of a randomized numerical method

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Received June 29, 1993 / Revised version received July 26, 1994

Summary. We analyze a randomized algorithm for solving the initial value problem for the finite dimensional system

$$\frac{dy}{dt} = f(t, y)\ ; \quad y(t_0) = y_0$$

on a finite interval under the hypothesis that f is smooth in y but no more than bounded and measurable in t. The algorithm is a representative member of an infinite family of methods akin to the Runge-Kutta family. It generates a sequence Y_k by iterating the single step formula

$$Y_1 = Y_0 + \frac{h}{2p}\sum_{j=1}^{p}\{f(U_j, Y_0 + hf(u_j, Y_0)) + f(u_j, Y_k)\}$$

$$U_j = \max(T_{1j}, T_{2j})\ , \quad u_j = \min(T_{1j}, T_{2j})$$

where for each step $\{T_{1j}\}$ and $\{T_{2j}\}$ are fresh p-fold random samples of the uniform distribution on $[t_0, t_0+h]$. We analyze the resulting random estimator Y of y by giving a weak law for its error that, with probability $1-\beta$, gives error bounds in terms of the parameters β, h and p.

Mathematics Subject Classification (1991): 34A50, 65C05, 621.20

1. Introduction

In [St] we have described a family of randomized numerical methods for solving the purely deterministic initial value problem for the finite dimensional system

$$\frac{dy}{dt} = f(t, y)\ ; \quad y(t_0) = y_0 \tag{1.1}$$

on a finite interval under the hypothesis that f is smooth in space (y) but no more than bounded and Borel measurable in time (t). This paper analyzes a probability model of a representative member of this family. This is a randomized single-step method which generates a sequence Y_k by

$$Y_{k+1} = Y_k + \frac{h}{p}\sum_{j=1}^{p}\left\{\frac{1}{2}f(U_{jk}, Y_k + hf(u_{jk}, Y_k)) + \frac{1}{2}f(u_{jk}, Y_k)\right\}$$

$$U_{jk} = \max(T_{1jk}, T_{2jk}), \quad u_{jk} = \min(T_{1jk}, T_{2jk}) \tag{1.2}$$

where for each step $\{T_{1jk}\}$ and $\{T_{2jk}\}$ are fresh p-fold random samples of the uniform distribution on the numerical grid interval $[t_k, t_k + h]$. Our main results describe the asymptotic form of the error and give a weak law (Theorem 2.4) which with proba bility $1 - \beta$ bounds the error in terms of β, h and p.

The entire infinite family is akin to the Runge-Kutta (RK) family [Bu] in its construction from self-substitutions of f and gives a rigorous technical form to the more or less obvious principle of averaging by randomization or hashing. The entire family, and also its relation to the RK family, can be nicely represented by the one-parameter subfamily of second order formulas

$$Y_1 = Y_0 + \frac{h}{p}\sum_{j=1}^{p}\left\{\frac{1}{2\alpha}f(U_{j0}, Y_0 + \alpha hf(u_{j0}, Y_0)) + \left(1 - \frac{1}{2\alpha}\right)f(u_j, Y_0)\right\}$$

where U_{j0} and u_{j0} are as given in (1.2). This resembles the simpler second-order RK formula

$$Y_1 = Y_0 + h\left\{\frac{1}{2\alpha}f(t_0 + \alpha h, Y_0 + \alpha hf(t_0, Y_0)) + \left(1 - \frac{1}{2\alpha}\right)f(t_0, Y_0)\right\}$$

(the formulas coincide if f is independent of t). However this latter formula generates a second order approximation to the solution of the differential equation only if f is differentiable in t. Since our problem does not allow reliance on smoothness in t, instead we discretize only with respect to the dependent variables, retaining dependence on t only through average or integral properties. This partial discretization combined with Monte-Carlo estimation of the remaining average t-dependence then yields numerical schemes that we have called Runge-Kutta Monte-Carlo (RKMC) algorithms. These unusual methods can enjoy some advantages compared to standard methods under two conditions. First, the problem should contain a discrepancy between the rates at which f varies in t and in y, the latter being significantly smaller in the natural scales of the problem than the former (a complete lack of regularity in t being essentially the most extreme case of this condition). Second, speed of integration should be important so that the speedup which can be gained by parallel calculation of the summands in the required Monte-Carlo estimations is of consequence. Under these conditions, comparisons on the basis of total computation time can sometimes show RKMC methods to advantage.

To show the character of RKMC methods and problems to which they are suited we will give an error analysis of the representative special case (1.2). But first, for illustration, we use the second order methods given above with $\alpha = 1$ to solve a simple problem with two grossly disparate scales:

$$\frac{dy}{dt} = y + \mu \sin(\cos(\lambda t)) \,, \quad y(0) = 1$$

where λ is large compared to μ, say $\lambda = 1023$ and $\mu = 5$. Calculating $y(t)$ up to $t = 1$ using the RK method with 10 and 100 equally spaced steps and the RKMC method with 10 equally spaced steps with $p = 100$ we find the result shown in Fig. 1.

Here the two RK integrations produce the visibly jagged curves. We have selected the parameters so that the integration with the larger time step is at the limit of its capacity to follow the solution. In contrast, the remaining relatively smooth curve, the result of the RKMC algorithm with the same number of time steps, follows the finer RK integration quite closely. This example, which depends smoothly (even analytically) on t, illustrates how the weak condition of bounded measurability can sometimes provide a reasonable mathematical model. Here smooth dependence on t is only visible as a rapid variation which for economic or other practical reasons (for example in the press of real-time calculation) we might be unable to follow in detail. It also illustrates concretely the significance here of the well-known parallelizibility of Monte-Carlo estimation. We also display $V(t)$ where $V^2(t)$ is the cumulative sample variance of the RKMC2 increments up to time t. The calculations displayed have been performed serially (in the Mathematica environment) but it is only because the p summands in (1.2) could have been evaluated in parallel with quite trivial overhead that the RKMC calculation can claim an advantage. In fact the RKMC calculation uses 1000 summand evaluations compared to 100 for the finer RK integration. Nevertheless since the 1000 can be executed in 10 time steps each containing 100, favorable comparison with each RK integration is justified, either on raw accuracy or on the total number of time steps.

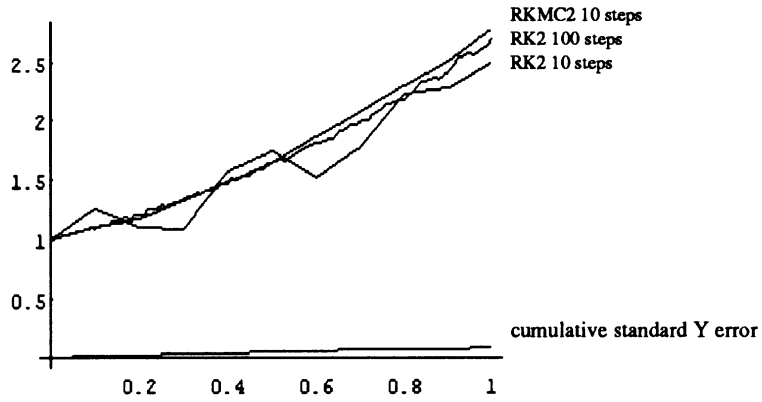

Fig. 1. $Y(t)$ vs t for RK2 with 10 and 100 steps and RKMC2 with 10 steps and $p = 100$ together with cumulative standard error in Y increments

Section 2 contains a precise formulation of our problem and states our main result. In Sect. 3 we recast the algorithm in a perturbation form. Section 4 proves preliminary deterministic estimates. Section 5 uses probabilistic reasoning to prove the main result. Methods of RK type for solving stochastic differential equations have been previously studied [So] but do not relate specifically to our problem. Also there is a vast literature for dynamical systems with random constituents giving, for example, many kinds of limit theorems. Since we are less interested in these than

in an asymptotic description of the error we prefer to derive a weak law *ab initio* by combining martingale estimates with standard classical deterministic perturbation arguments.

2. Hypotheses and main results

We proceed under hypotheses which generously ensure local existence and uniqueness for solutions. Moreover we are concerned only with approximating a given global solution $y(t)$ assumed to exist on a bounded time interval which without loss of generality we assume to be [0,1]. Since we are considering a second-order method, it is clear that the behavior of the algorithm must depend on local characteristics of $f(t,u)$ near the graph of $y(t)$ in $\mathbb{R}^{N+1}$ as embodied in the Taylor expansion with remainder

$$\begin{aligned} &f(t,y(t)+v) = f(t,y(t)) + f_y(t,y(t))v + f_2(t,v) \\ &\|f_2(t,v)\| \le M\|v\|^2 \end{aligned} \tag{2.1}$$

where $\|\ \|$ denotes the Euclidean norm on $\mathbb{R}^N$ and also the induced subordinate norms for linear operators and homogeneous polynomial forms.

Hypothesis 2.1. *There is an open neighborhood U in $\mathbb{R}^{N+1}$ of the graph of the solution $y(t)$ on which f and its y-partial derivatives up to order two are bounded and t-Borel measurable.*

We remark that if we understand solution as an absolutely continuous solution of

$$y(t) = y_0 + \int_{t_0}^{t} f(s,y(s))ds\ , \tag{2.2}$$

then this hypothesis easily brings the problem within the scope of local existence and uniqueness arguments by Picard iteration. It also ensures the existence of bounds for the norms of f, f_y, f_2 in expansion (2.1) which partially determine our error estimates. However we also require an additional measure of time conditioning or *local roughness in the scale of the computation* which depends both on the step size h and on subtler mean-quadratic properties of f near the solution.

Definition 2.2. Let $t_k = kh$, $y_k = y(t_k)$ and let E_k denote expectation with respect to the uniform distribution on $[t_k, t_{k+1}] \times [t_k, t_{k+1}]$. Let

$$F(t,s,u) = \frac{1}{2}\{f(\max[t.s], u + hf(\min[t,s],u) + f(\min[t,s],u)\}\ , \tag{2.3}$$

Let

$$\begin{aligned} &\sigma^2_{k+1}(h,u) = E_kE_k\left\{\|F(s_1,t_1,u) - F(s_2,t_2,u)\|^2\right\}\ , \\ &s^2_k(h) = \sup_{|u-y_{k-1}|\le d}\left\{\sigma^2_k(h,u)\right\}\ , \\ &S^2(t,h) = h\sum_{t_k\le t} s^2_k(h)\ . \end{aligned} \tag{2.4}$$

The quantities σ and s might appear to depend on f in an inaccessible way but in actual computation as an on-line practical estimate we have the sample variance

or standard error of the p evaluations of F required for a single time step. In the language of probability $\sigma^2(t_{k+1}, h, Y_k)$ is simply the conditional variance of $\frac{Y_{k+1}-Y_k}{h}$ given Y_k for which sample variance is the usual statistical estimator. In any case we always have the following crude estimate.

Lemma 2.3. *If* $\|f\| < M$ *then* $S \leq 2M$.

But if f has some regularity in t then we can sharpen this estimate. For example if f is actually differentiable then it is easy to see that $s = O(h)$.

In terms of this definition we can state our main result, the following weak law for Y_k which, in the language of probability, describes the uniform convergence in probability of all the Y_k to $y(t_k)$ as the numerical grid is refined.

Theorem 2.4 (Probabilistic Error Estimate). *There are positive constants* L *and* h_0 *such that, given a level* $\beta > 0$, *if*

$$\max\left[h, \left(\frac{h}{p\beta}\right)^{\frac{1}{2}} S(1,h)\right] < h_0$$

then with probability not less than $1-\beta$

$$\|Y_k - y(t_k)\| \leq L\left\{h^2 + \left(\frac{h}{\beta p}\right)^{\frac{1}{2}} S(t_k,h)\right\} .$$

According to this estimate describing the algorithm as "second order" is too simple although in the idealized situation where there is no limit on p, say $p = O(h^{-3})$, the global error is $O(h^2)$. The same estimate also follows from $p = O(h^{-1})$ if f is effectively smooth in the scale of the computation so that $S = O(h)$.

3. Small perturbation formulation

For convenience in notation let $y_k = y(t_k)$. As a basis for comparing the numerical and exact solutions we use the equation

$$y_{k+1} = y_k + \int_{t_k}^{t_{k+1}} f\left(t, y_k + \int_{t_k}^{t} f(s, y(s))ds\right) dt \tag{3.1}$$

which, as comparison with (1.2) suggests, is more closely related to the algorithm than Eq. (2.2). Then, recalling the definition of $F(t,s,u)$ in (2.3) and introducing p-fold random samples T_{1jk} and T_{2jk} of $[t_k, t_{k+1}]$ as in (1.2) we define

$$\begin{aligned} X_k &= \left(\frac{h}{p}\right)^{\frac{1}{2}} \left\{\sum_{j=1}^{p} F(T_{1jk}, T_{2jk}, Y_{k-1}) - pE_k(F(t,s,Y_{k-1})\right\} \\ W_0 &= 0 , \quad \text{and} \quad W_k = \sum_{0}^{k} X_k . \end{aligned} \tag{3.2}$$

Since the T_{ijk} are independent and uniformly distributed,

$$E\{X_k|W_1, W_2 \ldots W_{k-1}\} = E_k\{X_k) = 0$$

and the sequence W_k forms a martingale. In terms of W_k the numerical recursion can be expressed as

$$Y_{k+1} = Y_k + hE_k\{F(t, s, Y_k)\} + \left(\frac{h}{p}\right)^{\frac{1}{2}} (W_{k+1} - W_k) \tag{3.3}$$

which displays it, at least formally, as a small random perturbation of a deterministic recursion.

We next obtain an analogous recursion for the y_k.

Lemma 3.1. *$y_{k+1} = y_k + hE_k\{F(t, s, y_k)\} + h^3 G_k$ where $\|G_k\|$ is bounded.*

Proof. Expanding the inner and outer occurrences of f in (2.2) in its second argument about y_k and using bounds ensured by Hypothesis 2.1 we find

$$y_{k+1} = y_k + \int_{t_k}^{t_{k+1}} \left\{ f(t, y_k) + f_y(t, y_k) \int_{t_k}^{t} f(s, y(s))ds \right\} dt + O\{h^3) \ .$$

Interchanging the labels of the dummy variables and averaging gives

$$\begin{aligned} y_{k+1} = y_k + \frac{1}{2h} + \int_{t_k}^{t_{k+1}} \int_{t_k}^{t_{k+1}} \{f(t, y_k) + f(s, y_k)\} ds dt \\ + \int_{t_k}^{t_{k+1}} \int_{t_k}^{t} \frac{1}{2} f_y(t, y_k) f(s, y(s)) ds dt \\ + \int_{t_k}^{t_{k+1}} \int_{t_k}^{s} \frac{1}{2} f_y(s, y_k) f(t, y(s)) dt ds + O\{h^3) \ . \end{aligned}$$

Inverting order of integration on the last integral and introducing the lattice functions allows consolidation into

$$\begin{aligned} y_{k+1} = y_k + \frac{1}{2h} \int_{t_k}^{t_{k+1}} \int_{t_k}^{t_{k+1}} \{f(t, y_k) + f(s, y_k) \\ + h f_y(\max[s, t], y_k\} f(\min[s, t], y_k)\} ds dt + O(h^3) \ . \end{aligned}$$

Replacing $f(t, y_k) + f(s, y_k)$ by $f(\max[t, s], y_k) + f(\min[t, s], y_k)$ this then agrees to the indicated order with the Taylor expansion of

$$\begin{aligned} y_{k+1} = y_k + \frac{1}{2h} \int_{t_k}^{t_{k+1}} \int_{t_k}^{t_{k+1}} \{f(\max[s, t], y_k + h f(\min[s, t], y_k)) \\ + f(\min[s, t], y_k)\} ds dt + O(h^3) \ . \end{aligned}$$

This, restated in terms of $F(t, s, v)$ and expectation E_k with respect to the uniform density h^{-2}, is the desired conclusion. □

We now complete reformulation with the transformation

$$Y_k = y_k + \left(\frac{h}{p}\right)^{\frac{1}{2}} W_k + h^{\frac{1}{2}} Z_k \ . \tag{3.4}$$

In terms of Z_k , relation (3.3) and the lemma combine to recast the numerical recursion in the form

$$Z_{k+1} = Z_k + h^{\frac{1}{2}} E_k \left\{ F\left(t, s, y_k + \left(\frac{h}{p}\right)^{\frac{1}{2}} W_{k+1} + h^{\frac{1}{2}} Z_k\right) - F(t, s, y_k)\right\} - h^{\frac{5}{2}} G_k \ . \tag{3.5}$$

Again the perturbation character of this is only formal since W_k can be large. The remaining analysis will show that for small h this happens only with small probability.

4. Estimates under global hypotheses

First suppose that $f(t, .)$ is globally defined on $\mathbb{R}^N$ and that the bounds for the y-partial derivatives of Hypothesis 2.1 are also global. This is unnatural (it excludes even linear problems) but allows a useful preliminary step. Then we can continue the recursions for Y_k and W_k indefinitely so that (3.4) and (3.5) simply relate sequences which we know a priori to exist.

Definition 4.1. Given a sequence $\{H_j\}$ let $|||H|||_k = \max_{j\le k} \|H_j\|$.

Using this norm we can infer a bound for Z_k conditional on a bound for W_k uniform in h.

Lemma 4.2. *Given a norm bound B_0 for W_k uniform in k and h for $k < 1 + 1/h$ there are constants B_1 and h_0 such that for $h < h_0$ the sequence Z_k defined by (3.5) satisfies*

$$|||Z|||_k \le B_1 \left\{ h^{\frac{3}{2}} + p^{-\frac{1}{2}} |||W|||_k + h^{\frac{1}{2}} p^{-1} |||W|||_k^2 \right\} . \tag{4.1}$$

Proof. Taylor expansion of F with quadratic remainder in (3.5) implies there is C_1 such that

$$\|Z_{k+1}\| \le \|Z_k\| + C_1 h \left\{ \|Z_k\| + h^{\frac{1}{2}} \|Z_k\|^2 + p^{-\frac{1}{2}} \|W_{k+1}\| + h^{\frac{1}{2}} p^{-1} \|W_{k+1}\|^2 + h^{\frac{3}{2}} \right\} .$$

This implies that $\|Z_k\|$ is bounded by the solution of the scalar recursion

$$z_{k+1} = z_k + C_1 h \left\{ z_k + h^{\frac{1}{2}} z_k^2 + p^{-\frac{1}{2}} \|W_{k+1}\| + h^{\frac{1}{2}} p^{-1} \|W_{k+1}\|^2 + h^{\frac{3}{2}} \right\} .$$

This is equivalent to (using $z_0 = 0$, $W_0 = 0$)

$$z_{k+1} = \sum_{j=0}^{k} C_1 h (1 + C_1 h)^{k-j} \left\{ h^{\frac{1}{2}} z_j^2 + p^{-\frac{1}{2}} \|W_{j+1}\| + h^{\frac{1}{2}} p^{-1} \|W_{j+1}\|^2 + h^{\frac{3}{2}} \right\}$$

which implies, since $k < 1 + 1/h$, that there is C_2 for which

$$|||z|||_k \le C_2 \left\{ h^{\frac{1}{2}} |||z|||_k^2 + p^{-\frac{1}{2}} |||W|||_k + h^{\frac{1}{2}} p^{-1} |||W|||_k^2 + h^{\frac{3}{2}} \right\} .$$

Finally, the implicit function theorem and the smallness of the quadratic term for sufficiently small h yield a corresponding linear inequality of the desired form. □

To proceed further, still under global hypotheses, we introduce some probability theory.

Definition 4.3. Let $\mathscr{F}_k$ be the σ-field of events determined by the random variables $\{T_{ijk}\}$ appearing in the first k steps of algorithm (1.2) and let $\mathscr{F}_0$ be the trivial field.

The following is a direct consequence of the independence of the T_{ijk} and Definition 2.2.

Lemma 4.4.

$$\text{a)} \quad E\left\{\|W_k\|^2\right\} = \sum_{j=1}^{k} E\left\{\|X_j\|^2\right\} = \sum_{j=1}^{k} E\left\{E\left\{\|X_j\|^2 | \mathscr{F}_{j-1}\right\}\right\} ,$$

$$\text{b)} \quad E\left\{\|X_k\|^2 | \mathscr{F}_{k-1}\right\} = h\sigma_k^2(h) = S^2(t_k, h) - S^2(t_{k-1}, h) .$$

Lemma 4.5. *There is an $h_0 > 0$ such that if $h < h_0$ and $\|Y_k - y_k\| < d$ then*

$$E\left\{\|X_{k+1}\|^2 | \mathscr{F}_k\right\} \leq S^2(t_{k+1}, h) - S^2(t_k, h) .$$

Proof. The expectation is $h\sigma_{k+1}^2(h, Y_k)$ which by the constraint on Y_k and Definition 2.2 satisfies the stated estimate. □

5. Proof of main results

We now assume only that the derivative bounds for f hold only on a neighborhood of the graph of $y(t)$ in $\mathbb{R}^{N+1}$ and that d is chosen so small that sequences (t_k, u_k) satisfying $\|u_k - y_k\| < d$ lie in a smaller neighborhood with compact closure in the original neighborhood. Using the theory of martingales [D], chiefly Kolmogorov's inequality and stopping properties, we will show that the action of the algorithm can be constrained to this neighborhood with high probability. We use two devices to reduce the problem to the case with global bounds. First we extend f outside this smaller neighborhood to a globally defined function satisfying similar bounds everywhere. We then obtain modified processes which are defined for all time and satisfy the estimates of the previous section. The price that we pay for this extension is that we lose sight of an essential part of the process by altering paths of the original process which undergo large excursions. The second device is to further modify such paths by stopping them before such large excursions occur. The proof that for suitable h such stoppage is unlikely will be an application of the following basic results from the theory of martingales.

Lemma 5.1 ([D], [Br]). *Let $K = \{K_0, K_1, \ldots\}$.*

a) *If ϕ is convex and K is a martingale then $\phi(K)$ is a submartingale.*

b) *If k^* is a random index for which $\{k = k^*\}$ is $\mathscr{F}_k$-measurable and K is a martingale then K stopped at k^* is again a martingale.*

c) *(Kolmogorov's inequality) If K is a submartingale then*

$$P\left\{\max_{j \leq k} K_j > \varepsilon\right\} \leq \frac{1}{\varepsilon} E\{|K_k|\} .$$

Definition 5.2. Let k^* be the first entrance index of $\|Y_k - y_k\|$ into $[d, \infty)$ (or infinity if no entrance occurs). Let W^* be the process stopped at k^* and let X^*, Y^* and Z^* be the associated processes satisfying the stopped forms of relations (3.2), (3.3) and (3.4) so that, for example, $(X^*)_k = X_k$ unless $k > k^*$ in which case $(X^*)_k = 0$.

Lemma 5.3. $E\{\|(W^*)_k\|^2\} \leq S^2(t_k, h)$.

Proof. Define the process e^* by letting $(e^*)_k$ be the indicator function of $\{k^* \geq k\}$ for $k = 0, 1, \ldots$. Then the time history up to t_{k-1} determines $(e^*)_k$ so that $(e^*)_k$ is $\mathscr{F}_{k-1}$ measurable. Also $X^* = Xe^*$. Hence

$$E\left\{\|(X^*)_j\|^2 | \mathscr{F}_{j-1}\right\} = E\left\{\|X_j\|^2 (e^*)_j | \mathscr{F}_{j-1}\right\}$$
$$= (e^*)_j E\left\{\|X_j\|^2 | \mathscr{F}_{j-1}\right\} = (e^*)_j h\sigma_j^2(h) .$$

The stopping rule ensures that if $(e^*)_j$ is not 0 then $\|Y_{j-1} - y_{j-1}\| < d$. Thus in the stopped form of relation of Lemma 4.4a

$$E\left\{\|(W^*)_k\|^2\right\} = \sum_{j=1}^{k} E\left\{E\left\{\|(X^*)_j\|^2 | \mathscr{F}_{j-1}\right\}\right\}$$

the nonzero summands can be estimated according to Definition 2.2 by

$$E\left\{\|(X^*)_j\|^2 | \mathscr{F}_{j-1}\right\} \leq h s_j^2(h) = S^2(t_{j+1}) - S^2(t_j) .$$

Applying the expectation operator and summing completes the proof. □

Lemma 5.4.

$$P\left\{|||W^*|||_k \leq \beta^{-\frac{1}{2}} S(t_k, h)\right\} \geq 1 - \beta .$$

Proof. The stopped process W^* is again a martingale. Convexity of the square of the norm implies that $\|W^*\|^2$ is a submartingale. The estimate of Lemma 5.3 combined with Kolmogorov's inequality then gives the conclusion. □

Proof of Theorem 2.4. We confine our attention to the set of paths of probability at least $1-\beta$ on which $|||W^*|||_k \leq \beta^{-\frac{1}{2}} S(t_k, h)$. For such paths, the estimate of Lemma 4.2 gives

$$|||Z^*|||_k \leq B_1 \left\{h^{\frac{3}{2}} + (\beta p)^{-\frac{1}{2}} S(t_k, h) + h^{\frac{1}{2}} (\beta p)^{-1} S(t_k, h)^2\right\} .$$

By (3.4) this translates into an error estimate for the stopped process

$$\|(Y^*)_k - y_k\| \leq B_1 \left\{h^2 + \left(\frac{h}{p\beta}\right)^{\frac{1}{2}} S(t_k, h) + \frac{h}{p\beta} S(t_k, h)^2\right\} .$$

By Lemma 2.3, S has a bound depending only on f. Also, since $(\frac{h}{\beta p})^{\frac{1}{2}} S < h_0$, we can absorb the quadratic term in S into the linear to obtain an estimate of the stated form. Finally, for h_0 small enough, it follows that the error und for Y is smaller than d and hence that all the evaluations of f appearing in recursion (3.5) occur near the graph of y where our global modification of f agrees with the original f. Such

paths are unstopped and constitute a set of paths of the original algorithmic process satisfying the estimate of the theorem with the required probability. □

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