

Computing exit times with the Euler scheme

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Abstract

In this note we study standard Euler updates for computing first exit times of general diffusions from a domain. We focus on one dimensional situations and show how the ideas of Mannella and Gobet can be adapted to this problem. In particular, we give a fully implementable algorithm to compute the first exit time from an interval numerically. The Brownian motion case is treated in detail.

Special emphasize is on numerical experiments: For every ansatz, we include numerical experiments confirming the conjectured accuracy of our methods. Our methods appear to be at least of weak order one and give improved results at the same computational cost compared to algorithms used widely in practice.

1 Introduction

1.1 Problem formulation

Computing the first exit time of a stochastic process from a domain with high accuracy is of significant interest in many applications. Examples range from financial derivatives with barriers to path integrals in mathematical physics. Here, we discuss the probabilistic solution of Dirichlet problems. If one applies the Feynman-Kac formula to get a probabilistic representation of the solution to a certain Dirichlet problem, the first exit time plays a crucial role. There, one integrates along a path until this path leaves the domain for the first time. In more detail, let D be a bounded domain in n -space with smooth boundary ∂D and consider the following boundary value problem (BVP). We focus on the Poisson equation for its simplicity:

$$\frac{1}{2} \Delta u(x) + g(x) = 0, \quad x \in D, \quad u(x) = \psi(x), \quad x \in \partial D. \quad (1)$$

Then, the solution $u(x)$ is given by the Feynman-Kac formula (under some regularity and smoothness conditions on g , ψ and D (see for example [Fre85])),

$$u(x) = \mathbb{E}_x \left[\psi(X(\tau)) + \int_0^\tau g(X(s)) ds \right], \quad (2)$$

where

$$X(t) = x + \int_0^t dW(s). \quad (3)$$

We introduced in (2) the first exit time of $(X(t))_{t \geq 0}$ from D (or, by continuity, the first passage time to ∂D), $\tau = \tau(x)$,

$$\tau(x) = \inf\{t > 0 : X(t) \notin D\} = \inf\{t > 0 : X(t) \in \partial D\}, \quad X(0) = x. \quad (4)$$

$X(t)$ is a Brownian motion starting at x . The starting point, x , also appears in the symbol \mathbb{E}_x for the expectation and will show up again when we denote densities, distributions or general probabilities as \mathbb{P}_x . We implicitly assume $x \in D$. Approximating $u(x)$ numerically using the representation (2) is in principle straightforward: One introduces $f(t) = \int_0^t g(X(s)) ds$ and considers the system of stochastic differential equations (SDEs)

$$dX = dW \quad \text{and} \quad df = g(X) dt \quad \text{with} \quad X(0) = x \quad \text{and} \quad f(0) = 0. \quad (5)$$

System (5) is then integrated numerically for a (large) number, say N , of paths, and the expectation in (2) is approximated by the mean over these N independent realizations.

The Euler scheme (or Euler-Maruyama scheme), due to its simplicity, is of great interest. Applied to system (5) with a fixed time step of size h , it takes the form

$$X_{k+1} = X_k + \Delta W_k \quad \text{and} \quad f_{k+1} = f_k + g(X_k)h \quad (k = 0, 1, \dots), \quad (6)$$

with $X_0 = x$ and $f_0 = 0$. Here, an n -vector, ΔW_k , of i.i.d. normal random variables with mean 0 and variance h is generated in each time step. We denote such random variables by the symbol \mathcal{N}_0^h . Additionally, we will use the symbol \mathcal{U} for random variables distributed uniformly in $(0, 1)$.

The main difficulty presents itself: when should the (numerical) integration be stopped? In other words: How shall $X(\tau)$ and in particular τ be approximated? We concentrate on the approximation of τ in this note, corresponding to a constant boundary condition ψ in (1).

The naive approach is to stop as soon as $X_k \notin D$ and to take as an approximation for the first exit time $\tau \approx (k-1)h$, $\tau \approx kh$ or a certain value between these two values.

We compare our results in the case $\psi \equiv 0$ in (1) to

Algorithm 1 (naive Euler) Update according to (6) until $X_{k+1} \notin D$. Approximate $f(\tau) \approx f_k$.

The drawback of this approach is the loss of accuracy: Although the Euler scheme is of weak order one for a fixed final time T with $M + 1$ discretization points (giving $h = T/M$ in our notation, see for example [KP92]), the rate of convergence in the weak sense in the presence of a boundary reduces to $\mathcal{O}(\sqrt{h})$, i.e. it is of weak order one half [Gob00]. The reason for this loss of accuracy is as follows: Although the discrete random walk is correct in distribution sense ($X((k + 1)h) - X(kh) \stackrel{law}{=} X_{k+1} - X_k \stackrel{law}{=} \mathcal{N}_0^h$ in one dimension and the same holds for any component in higher dimensions) it gives the process values only at discrete time points $t_k = kh$. In between, for $t_k < t < t_{k+1}$, we have no information on the behaviour of the continuous process $X(t)$. Both Mannella and Gobet pointed out (see also Janson and Lythe [JL00]) that anywhere near the boundary the process might have left D and come back within step h : Even if both X_k and $X_{k+1} \in D$, it is not unlikely that $X(t) \notin D$ for some $t \in (t_k, t_{k+1})$ – the process $X(t)$ might follow an excursion within h , implying $\tau < t_{k+1}$.

Remark 1 *It is clear from above reasoning that Algorithm 1 will overestimate τ , as no intermediate excursions are monitored.*

Mannella proposed a simple hitting test in [Man99] to be performed after each time step with $X_{k+1} \in D$. This test estimates the probability that an excursion occurred and leads to improved statistics. Gobet later proved that first order weak convergence can be obtained for the Euler scheme when applying this test for *killed* diffusions in the presence of a boundary. For fixed $T < \infty$, paths for which $\tau < T$ are killed, that is, they do not contribute to the expectation.

The purpose of this note is to show how these ideas might be applied to the case of stopped (rather than killed) diffusions. In this case, one is interested in the actual value of τ rather than being satisfied by the assertion that (or if) $\tau < T$ for some predefined (deterministic) T . In other words, one wants to know (again in a statistical sense) *when* the first exit time actually took place rather than asking only *if* the exit did already occur. We show how a new interpretation of the exit probability as a distribution leads to more accurate results (yet of the same order) for exactly the same computational cost. We then further improve our algorithm for a Brownian motion for the case that a discrete X_k falls outside D . Our numerical tests show that we are left almost with the statistical error – keeping the systematic error tiny.

1.2 The main test problem

Throughout the paper, we include results for the different algorithms applied to our main test problem. To test the different approaches we suggest the following simple problem: Set in the boundary value problem (1) $g \equiv 1$ and $\psi \equiv 0$. Then by (2) $u(x) = \mathbb{E}_x[\tau(x)]$. For $n = 1$, the solution for $D = (\alpha, \beta)$ is then

$$u(x) = -x^2 + (\alpha + \beta)x - \alpha\beta. \quad (7)$$

We summarize in

Test problem 1 (Main test problem) *In $n = 1$ we consider in $D = (\alpha, \beta)$ with $\alpha < 0 < \beta$ the BVP (1) with $g \equiv 1$ and $\psi \equiv 0$. Our test measurement will be $u(0) \stackrel{(7)}{=} -\alpha\beta$.*

Note that the Euler scheme (6) is exact in distribution for both X and f in system (5) with $g(x) \equiv 1$ as all the higher order terms in an Itô-Taylor expansion vanish. The updates take the simple form $X_{k+1} = X_k + \mathcal{N}_0^h$, $f_{k+1} = f_k + h$. The only errors besides statistical ones are those due to the approximation of $\tau(x)$ – the variable of interest.

1.3 Organisation of the paper

Clearly, the Feynman-Kac formulation (2) reveals its full strength mainly (but not only) in high dimensions. Nevertheless, we concentrate on a simple one dimensional problem here, in particular we shall consider $D = (\alpha, \beta)$ with $-\infty < \alpha < \beta < \infty$. The justification for this simplification is twofold: (i) the simple one dimensional situation is already interesting on its own and contains

the main difficulties, and, (ii) we hope to be able to apply a big part of the ideas presented here also in higher dimensions. If n becomes large, the domains D are usually smooth with boundaries. Near to the boundary it looks flat. There, locally, the problem of a random walk approaching the boundary resembles to some extent the one dimensional situation. Gobet on the other hand, approximated quite general domains in n -space locally as a half space if the walk is close to the boundary. He then presented formulae for general $n > 1$ [Gob00].

In Section 2 we recall the main idea of an exit test of Mannella and Gobet for killed diffusions. In Section 3 we show a simple improvement for the case of stopped diffusions which improves results at exactly the same cost (Subsection 3.1). For the pure Brownian motion ($dX = dW$) we improve these results further (Subsection 3.2). In Section 4 we extend the ideas presented so far to the case of more general diffusions which arise for more general (elliptic) operators in the Feynman-Kac formulation and show a general numerical test. Throughout the paper we include results of numerical experiments.

2 The ideas of Mannella and Gobet

As mentioned in Section 1 we restrict our work to the case $n = 1$. We start with some notation and known formulae (see [BS02] and consider some basic probability manipulations).

2.1 Notation and formulae

Let

$$S_t(x) = \sup_{0 \leq s \leq t} X(s), \quad X(0) = x.$$

We further introduce the first hitting time of level B as

$$H_B(x) = \inf\{t \geq 0 : X(t) = B\}, \quad X(0) = x. \quad (8)$$

We have for $y, z \leq B$

$$\mathbb{P}_y[H_B(y) \leq t, X(t) \in dz] = \mathbb{P}_y[S_t(y) \geq B; X(t) \in dz] = \exp\left(-\frac{2(B-y)(B-z)}{t}\right). \quad (9)$$

Let $X^{y,h,z}(t)$ be a Brownian bridge starting at $t = 0$ at y and ending at $t = h$ at z (i.e. the bridge is pinned in time-space coordinates at $(0, y)$ and at (h, z) and has $\mathbb{E}_y[X^{y,h,z}(t)] = y + (z - y)t/h$ and $Cov(X^{y,h,z}(t), X^{y,h,z}(s)) = (s \wedge t) - st/h$ [IW89]). Denote its law by $\mathbb{P}_{y,h,z}[\cdot]$. Then we might write (assuming $B \geq y$ and using (9))

$$\mathbb{P}_{y,h,z}[H_B(y) \leq h] = \begin{cases} 1, & y \leq B \leq z \\ \exp\left(-\frac{2}{h}(B-y)(B-z)\right), & y, z \leq B. \end{cases} \quad (10)$$

On the other hand, for $D = (\alpha, \beta)$ we have (see 4) $\tau = H_\alpha \wedge H_\beta$. For $\alpha < y, z < \beta$ it is known that [Gob00, RY91]

$$\begin{aligned} \mathbb{P}_{y,h,z}[\tau(y) \leq h] &= \sum_{k=-\infty}^{k=\infty} \left\{ \exp\left(-\frac{2}{h}k(\beta-\alpha)(k(\beta-\alpha) + z - y)\right) \right. \\ &\quad \left. - \exp\left(-\frac{2}{h}(k(\beta-\alpha) + y - \beta)(k(\beta-\alpha) + z - \beta)\right) \right\}. \end{aligned} \quad (11)$$

Again, clearly $\mathbb{P}_{y,h,z}[\tau(y) \leq h] = 1$ if any $y, z \notin D$. Clearly, in the case of an excursion, the formula (10) for H_B is much simpler to evaluate than formula (11) for τ .

2.2 The main idea

The idea for killed diffusions according to Gobet is as follows. Assume $X_k = y \in D$, $t_k + h < T$ and generate an Euler update as $X_{k+1} = y + \mathcal{N}_0^h = z$. Now there are two cases: (i) $z \notin D$ and (ii) $z \in D$. In the first case, $X(t)$ clearly left the domain and this path is killed (as $\tau < T$). On the other hand in the case (ii), one has to account for the possibility that the continuous path left D and came back. To this end, a test according to (10) or (11) is performed. Clearly, test (11) would be the correct one for $D = (\alpha, \beta)$. On the other hand, (10) is much simpler and much cheaper to calculate on a computer. Moreover, in higher dimensions, closed formulas of the form (11) are only known for half spaces. Assume now that $h \ll 1$ such that $\sqrt{h} \ll |\beta - \alpha|$, i.e. the average size of the space increments is much smaller than the diameter of the domain. Then, the probability that the path follows an excursion within h and came back has a value sufficiently large to be taken into account only if the boundary is sufficiently close. Therefore, the test (10) is applied only for the *closest* boundary. If h is sufficiently small (such that $\sqrt{h} \ll |\beta - \alpha|$), the resulting error in doing so is very small compared to the reduction in computer time (which could be used to reduce the overall error by choosing a smaller stepsize h or a larger sample N).

In more detail, for $y, z \in D = (\alpha, \beta)$ we define the closest boundary B as follows. Let $\rho_\alpha = (y - \alpha) \wedge (z - \alpha)$ and $\rho_\beta = (\beta - y) \wedge (\beta - z)$. If $\rho_\alpha < \rho_\beta$ we set $B = \alpha$ and $B = \beta$ otherwise. The event that both boundaries are equally far away has probability zero in theory and an almost vanishing probability on a computer. Additionally, in that case either $y = z$ (with probability zero) or y and z are symmetric wrt. the point $(\alpha + \beta)/2$. In the latter case, both boundaries are far away, and the exit probability goes to zero. The error arising if we set $B = \beta$ in these worst case situations is therefore negligible.

To evaluate expectations over functionals F of the form $\mathbb{E}_x[F(X_T)\mathbf{1}_{T < \tau}]$ the approach of Gobet for the Euler scheme is the following. After an update of the form (6), set $X_k = y$, $X_{k+1} = z$. In the case that $z \in D$, generate a random variable \mathcal{U} uniform in $(0, 1)$. If $\mathcal{U} \leq \mathbb{P}_{y,h,z}[H_B(y) \leq h]$, the path is deemed to have left D across B within h and the diffusion is killed. Gobet proved that if F is bounded and of class $C^3(\overline{D}, \mathbb{R})$, $T < \infty$ fixed and $h = T/M$, convergence is of weak order one (for fixed T) whereas the Algorithm 1 converges with $\mathcal{O}(\sqrt{h})$.

Applying these ideas to functionals of the form $u(x) = \mathbb{E}_x[f(\tau)]$ (see (2) with $\psi \equiv 0$) is straight forward: Assume again $X_k = y \in D$ and $z = X_k + \mathcal{N}_0^h$ and that B is the closest boundary.

Algorithm 2 (Gobet test) *If $z \notin D$ or $\mathcal{U} < \mathbb{P}_{y,h,z}[H_B(y) \leq h]$ we stop the integration at t_k and have for this path $f(\tau) \approx f_k$. Otherwise, we update $f_{k+1} = f_k + hg(X_k)$ and $X_{k+1} = z$.*

Remark 2 *Algorithm 2 will certainly underestimate τ , as the exit time will be set to t_k if an excursion occurred before t_{k+1} (but after t_k). In the case $z = X_{k+1} \notin D$, we approximate $\tau \approx t_k$, although the true exit took place in both cases at a time t **between** t_k and t_{k+1} .*

Remark 3 *Another advantage of applying a test according to (10) instead of (11) shows up in the case of non-constant $\psi(\cdot)$: In the case of an excursion across the closest boundary B , $\psi(B)$ might be used for the evaluation of functional (2) for the corresponding path, i.e. $X(\tau) \approx B$.*

2.3 Numerical experiments

We show results which confirm the conjectured first order in weak convergence. To see if the application of the test (10) instead of (11) is admissible, we set $\beta = 1$ and took three different values for the lower boundary, namely $\alpha = -7, -3, -1$. We applied Algorithm 2 to the Problem 1. In the plot of the absolute error $|u(0) - \hat{u}(0)|$ we add a 66%-confidence interval $\hat{\sigma}$ (numerical standard deviation),

$$\hat{\sigma}(\hat{u}) = \sqrt{\frac{\hat{u}^2 - \bar{u}^2}{N-1}} \quad \text{with} \quad \bar{u}^2 = \frac{1}{N} \sum_{i=1}^N (\hat{u}^{(i)})^2 \quad \text{and} \quad \bar{u} = \frac{1}{N} \sum_{i=1}^N \hat{u}^{(i)} \quad (12)$$

where $\hat{u}^{(i)}$ denotes the result obtained for sample i , $i = 1, \dots, N$. Results in Figure 1 are for a sample size of $N = 10^6$ on the left and for $N = 4 \cdot 10^6$ on the right. We used the random number

generator *Mersenne Twister* from the blitz-library [Vel98] for the exit test (10) and to generate the normal increments $\Delta W \stackrel{\text{law}}{=} \mathcal{N}_0^h$. In all our tests we used this random number generator. The maximal stepsize is $h_{max} = (\beta - \alpha)/4$ and we show results for h_{max} and seven smaller stepsizes.

Error $|\hat{u}(0) - u(0)|$ and $\hat{\sigma}$ vs. stepsize h for $\alpha = -7, -3, -1$ and $\beta = 1$.

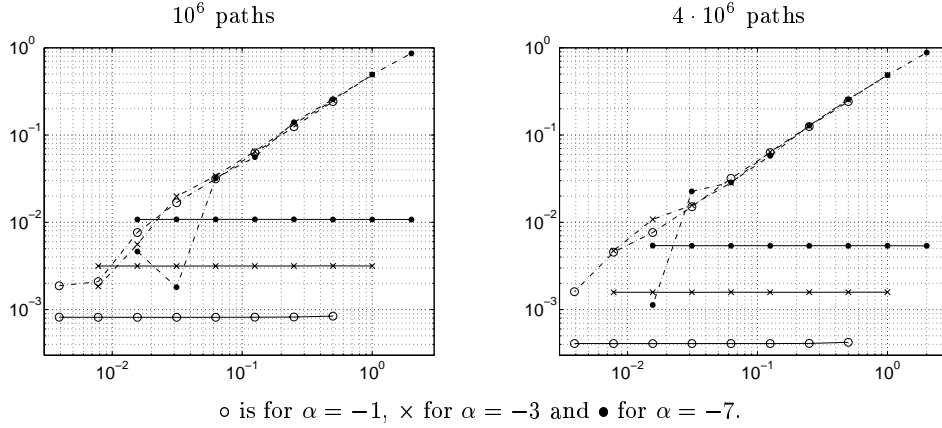
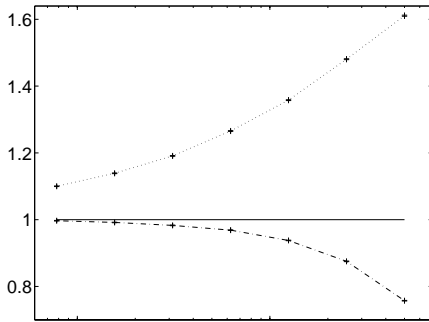


Figure 1: Testing only for the closest boundary preserves weak order one.

From Figure 1 it can be seen, that the weak order of convergence is $\mathcal{O}(h)$ independent of the choice of α . Note that decreasing α (and hence increasing the size of the domain) increases $\hat{\sigma}$ as on average more steps are needed till a path is stopped (the expected exit time increases).

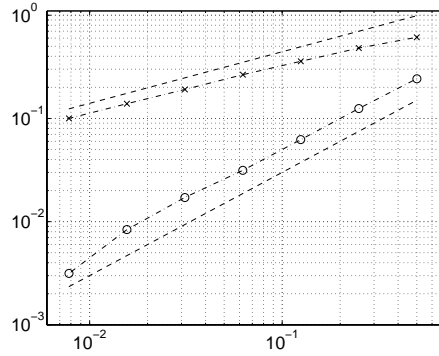
In the next figure (Figure 2) we have a closer look at the solution $\hat{u}(0)$ for $D = (-1, 1)$. We compare the naive approach (Algorithm 1) with the straight forward application of the ideas recited in this section (Algorithm 2). We have $u(0) = 1$ (indicated by a solid line) and show results for $N = 10^6$ paths. The remarks made before (Remarks 1 and 2) are very obvious in this plot.

Solutions $\hat{u}(0) \pm \hat{\sigma}(\hat{u}(0))$ vs stepsize h .



——— is $u(0) = 1$
 is Algorithm 1
 - - - is Algorithm 2

Error $|\hat{u}(0) - u(0)|$ vs. stepsize h .



- · × · - is Algorithm 1
 - · o · - is Algorithm 2
 - - - have slope 1/2 and 1

Figure 2: Algorithm 1 overestimates $\mathbb{E}_0[\tau] = 1$ whereas Algorithm 2 underestimates it. Weak order of convergence improves from $\mathcal{O}(\sqrt{h})$ (for Algorithm 1) to $\mathcal{O}(h)$ (for Algorithm 2).

3 Improvements

In this section we present an extension to Algorithm 2 which gives a better approximation of $\tau \in (t_k, t_{k+1})$. To simplify notation we assume $X_k = y \in D$ and set $X_{k+1} = X_k + \mathcal{N}_0^h = z$ throughout this Section. Without loss of generality we assume that $\beta > 0$ is the closest boundary, i.e. $B = \beta > y$. The situation $B = \alpha < y$ is obtained by symmetry.

3.1 The case $X_k = y \in D$ and $X_{k+1} = z \in D$

The first improvement is based on a new interpretation of $\mathbb{P}_{y,h,z}[H_\beta(y) \leq h]$ as the distribution of the first hitting time of level β (see (10)). It gives an improvement in the error of a factor of two at exactly the same computational cost (preserving the order of convergence) when applied to Problem 1 in $D = (-1, 1)$.

3.1.1 Generate $\mathcal{H} \stackrel{\text{law}}{=} \mathbb{P}_{y,h,z}[H_\beta(y) \leq t]$

For $y, z < \beta$, we are in particular interested in $\mathbb{P}_{y,h,z}[H_\beta(y) \leq h]$. On the other hand, this gives us the distribution, F , of the first hitting time wrt. Brownian bridge measure (see (10))

$$F_{H_\beta(y)}^{y,h,z}(t) \equiv \mathbb{P}_{y,h,z}[H_\beta(y) \leq t] = e^{-\frac{1}{2t}(\beta-y)(\beta-z)} \mathbf{1}_{t \geq 0}, \quad y, z \leq \beta. \quad (13)$$

The idea is now to generate a random variable \mathcal{H} with distribution (13). To this end, invert (13) [KP92, p.12],

$$\mathcal{H} = -\frac{2(\beta-y)(\beta-z)}{\log \mathcal{U}} \quad (14)$$

where \mathcal{U} is again a uniform random number in $(0, 1)$. The path hit β between t_k and $t_{k+1} = t_k + h$ if $\mathcal{H} \leq h$ (in a statistical sense). In that case, β was hit for the first time at $t = t_k + \mathcal{H}$ and we add a last Euler step with length \mathcal{H} to f :

$$f(\tau) = \int_0^\tau g(X(s))ds \stackrel{\text{law}}{=} \int_0^{t_k} g(X(s))ds + \int_{t_k}^{\mathcal{H}} g(X(s))ds \stackrel{(6)}{\approx} f_k + \mathcal{H}g(X_k).$$

Summarizing, we get

Algorithm 3 (Simulating the distribution in the case $y, z \in D$) *If $z \notin D$ we stop the integration at t_k . If $z \in D$ and $\mathcal{H} \leq h$ (where \mathcal{H} is generated according to (14)) we add a last Euler step of length \mathcal{H} to f and stop: $f(\tau) \approx f_k + \mathcal{H}g(X_k)$. Otherwise, we update $f_{k+1} = f_k + hg(X_k)$ and $X_{k+1} = z$.*

Remark 4 *Clearly, generating (14) is not more costly than generating \mathcal{U} and evaluating (10) as in Algorithm 2.*

3.1.2 Numerical experiment

We consider again $D = (-1, 1)$ and compare Algorithms 2 and 3 applied to Problem 1. As in Figure 2 we show the approximation $\hat{u}(0) \pm \hat{\sigma}(\hat{u}(0))$ and the error $|\hat{u}(0) - u(0)|$ for a sample of $N = 10^6$ paths.

Looking at Figure 3 it is evident that results improve. For Problem 1 with $D = (-1, 1)$ we observed in our experiments an improvement in the error by approximately a factor of two (of course, only in the regime where h is big enough such that the systematic error dominates and the statistical error of $\mathcal{O}(1/\sqrt{N})$ is negligible), see Table 1. Results were rounded to five significant digits.

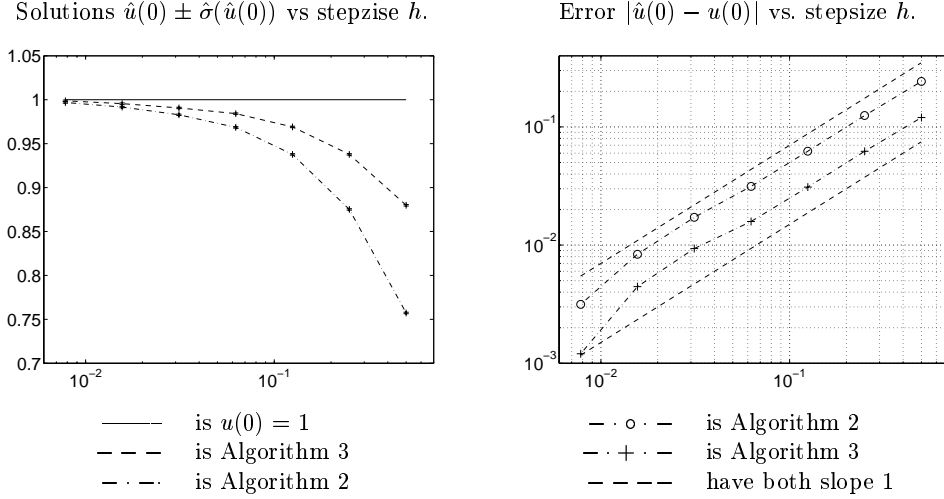


Figure 3: Generating a random number \mathcal{H} improves results by a factor of two at the same cost.

$k, h = 2^{-k}$	Error $ \hat{u}(0) - u(0) $	
	Algorithm 2	Algorithm 3
1	0.24273	0.12011
2	0.12485	0.062221
3	0.062285	0.030980
4	0.031433	0.015837
5	0.017166	0.0093502

Table 1: Algorithm 3 improves results compared to Algorithm 2 at the same cost.

3.2 The case $X_k = y \in D$ and $X_{k+1} = z \notin D$

Let

$$p(t; x, y) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{(x-y)^2}{2t}\right).$$

Using absolute continuity of the measures \mathbb{P}_y and $\mathbb{P}_{y,h,z}$ we have [BS02, p.67]

$$\mathbb{P}_{y,h,z}[H_\beta(y) \leq h] = p(h; y, z)^{-1} \int_0^h p(h-t; b, z) \mathbb{P}_y[H_\beta(y) \in dt]$$

with (see for example [RW00, (13.5), p.26])

$$\mathbb{P}_y[H_\beta(y) \in dt] = \frac{|\beta - y|}{t\sqrt{2\pi t}} \exp\left(-\frac{(y - \beta)^2}{2t}\right) dt.$$

Together,

$$\mathbb{P}_{y,h,z}[H_\beta(y) \leq h] = \frac{|\beta - y|}{\sqrt{2\pi}} \int_0^h \sqrt{\frac{h}{t^3(h-t)}} \exp\left(-\frac{1}{2} \left(-\frac{(z-y)^2}{h} + \frac{(\beta-z)^2}{h-t} + \frac{(\beta-y)^2}{t} \right)\right) dt.$$

Recall our assumption $y < \beta < z$ and introduce the shorthands $\tilde{\beta} = \beta - y$, $\tilde{z} = z - y$ and $\tilde{t} = t/h$. With these notations, after arranging the terms in the exponent we find

$$\mathbb{P}_{y,h,z}[H_\beta(y) \leq h] = \frac{\tilde{\beta}}{\sqrt{2\pi h}} \int_0^1 \frac{1}{\sqrt{\tilde{t}^3(1-\tilde{t})}} \exp\left(-\frac{1}{2h} \frac{(\tilde{\beta} - \tilde{t}\tilde{z})^2}{\tilde{t}(1-\tilde{t})}\right) d\tilde{t}. \quad (15)$$

As we did not succeed in calculating and inverting $\mathbb{P}_{y,h,z}[H_\beta(y) \leq t]$ for $0 \leq t \leq h$ we use some approximations for the statistics of $H_\beta(y)$. They are given in the following paragraphs and will be denoted by \hat{H} . We then get the final algorithm, which is based on Algorithm 3. Again, $y = X_k$ and $z = X_{k+1}$.

Algorithm 4 (Approximations in the case $z \notin D$) *If $z \in D$ we proceed as in Algorithm 3. If $z \notin D$ we calculate \hat{H} for the closest boundary according to (16) or (17) or generate it according to (19). Then, we add a last Euler step of length \hat{H} to f : $f(\tau) \approx f_k + \hat{H}g(X_k)$.*

3.2.1 Choosing the peak

As a first approximation, we choose the $t \in (0, h)$ where the density of the hitting time of β is maximal,

$$\hat{H}_{peak} = \arg \max_{t \in (0, h)} \frac{\mathbb{P}_{y,h,z}[H_\beta(y) \in dt]}{dt}. \quad (16)$$

The calculation of \hat{H}_{peak} reduces to find the roots of a cubic polynomial. For completeness, it is given in Appendix A.

3.2.2 Heuristic approximations

We compare the approach from Section 3.2.1 with two heuristic approximations.

Linear interpolant Here we choose the linear interpolant as an approximation for $H_\beta(y) \in (0, h)$, namely

$$\hat{H}_{lip} = h \frac{\beta - y}{z - y}. \quad (17)$$

This approach is justified by a result which is interesting on its own and shall be given in a little lemma.

Lemma 1 *Fix $y = X_k$ and $z = X_{k+1}$ and assume $y < \beta < z$. Then, the expectation $\mathbb{E}_{y,h,z}[H_\beta(y)]$ is a linear function of $\beta - y$, i.e.*

$$\mathbb{E}_{y,h,z}[H_\beta(y)] = C(\beta - y) \quad (18)$$

where C depends only on the distance $X_{k+1} - X_k$ and the timestep h .

The proof is given in Appendix B.

Uniform distribution Another heuristic approach is a uniform random variable, i.e.

$$\hat{H}_{uni} = h\mathcal{U} \quad (19)$$

ignoring the location of the boundary β within y and z completely.

3.2.3 Numerical experiment

We consider again Problem 1 with $D = (-1, 1)$. Applying Algorithm 4 leads to very small errors – independent of the approximation chosen for \hat{H} . We therefore show simulations with three different (large) sample sizes N . Above the approximations $\hat{u}(0)$ are shown (confidence levels $\hat{\sigma}$ are smaller than the plot symbols) and below the errors $|\hat{u}(0) - u(0)|$.

Figure 4 leads to the following heuristic conclusions: the two approximations (16) and (17) conserve the weak order of convergence of $\mathcal{O}(h)$ but with a smaller constant than application of Algorithms 2 and 3. The uniform approximation (19) has a smaller error, but it has to be noted that it is more costly to generate \mathcal{U} than evaluating for example the simple expression (17). From the proof in Appendix B we also see the reason, why linear interpolation (17) is overestimating the solution: this approximation corresponds to the choice $C = 1$ in (18), which is only true for $z \gg y$. Convergence of the approximation (19) is very fast and one has almost only the statistical error.

Solutions $\hat{u}(0)$ vs. stepsize h on top and error $|\hat{u}(0) - u(0)|$ vs. h on bottom.

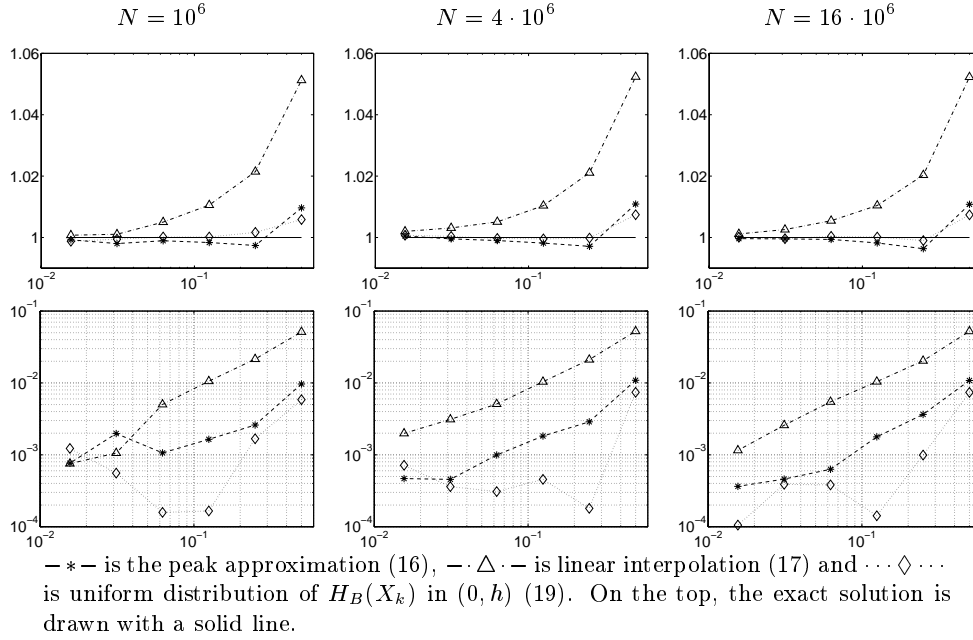


Figure 4: Adding a correction in the case $X_{k+1} \notin D$ improves results and errors become very small.

4 Extension to more general diffusions

In this section we extend the ideas presented so far to more general BVPs which lead to general diffusions. Again, we limit ourselves to a one dimensional situation.

4.1 The general Dirichlet problem

Let $D = (\alpha, \beta)$ and consider a generalization of (1)

$$\left[\frac{1}{2}a(x) \frac{d^2}{dx^2} + b(x) \frac{d}{dx} \right] u(x) + g(x) = 0, \quad x \in D, \quad u(x) = \psi(x), \quad x \in \partial D \quad (20)$$

where $a(x) > 0$. The probabilistic solution is again given by (2) where now (compare with (3))

$$X(t) = x + \int_0^t b(X(s)) ds + \int_0^t \sigma(X(s)) dW(s) \quad (21)$$

with $\sigma^2(x) = a(x)$. Numerically, we shall now solve (compare with (5))

$$dX = b(X) dt + \sigma(X) dW \quad \text{and} \quad df = g(X) dt \quad \text{with} \quad X(0) = x \quad \text{and} \quad f(0) = 0. \quad (22)$$

The corresponding Euler approximation is (compare with (6))

$$X_{k+1} = X_k + b(X_k)h + \sigma(X_k)\mathcal{N}_0^h \quad \text{and} \quad f_{k+1} = f_k + g(X_k)h \quad (k = 0, 1, \dots) \quad (23)$$

where we set as before $X_0 = x$ and $f_0 = 0$.

4.2 Extending Algorithms 2 and 3

Let $y = X_k$ and denote by z the next Euler update obtained using (23): $z = X_{k+1}$. Assume $y, z < B$ where B denotes again the closest boundary. The counterpart of (9) is [Gob00]

$$\mathbb{P}_y [H_B(y) \leq t; X(t) \in dz] = \exp\left(-\frac{2(B-y)(B-z)}{t\sigma^2(y)}\right). \quad (24)$$

Inverting (24) leads to (compare with 14)

$$\mathcal{H} = -\frac{2(B-y)(B-z)}{\sigma^2(y) \log \mathcal{U}} \quad (25)$$

where \mathcal{U} is again a uniform random number in $(0, 1)$.

The adaption of Algorithm 2 is now obvious:

Algorithm 5 (Gobet test for general diffusions) *Let $y = X_k$ and $z = X_{k+1}$. If $z \notin D$ or*

$$\mathcal{U} < \exp\left(\frac{-2(B-y)(B-z)}{h\sigma^2(y)}\right)$$

we stop the integration at t_k and set for this path $f(\tau) \approx f_k$. Otherwise, we update $f_{k+1} = f_k + hg(X_k)$ and $X_{k+1} = z$.

Algorithm 3 is adapted similarly:

Algorithm 6 (Simulating the distribution in the case $y, z \in D$ for general diffusions) *If $z \notin D$ we stop the integration at t_k and set $f(\tau) \approx f_k$. If $z \in D$ and $\mathcal{H} \leq h$ (where \mathcal{H} is generated according to (25)) we add a last Euler step of length \mathcal{H} to f and stop: $f(\tau) \approx f_k + \mathcal{H}g(X_k)$. Otherwise, we update $f_{k+1} = f_k + hg(X_k)$ and $X_{k+1} = z$.*

4.3 Numerical experiment

Test problem 2 (Test for generalized BVP) *We show results for the BVP (20) with*

$$\sigma(x) = 2 + \sin(x), \quad a(x) = \sigma^2(x), \quad b(x) = -\cos(x) \left(2 + \frac{\sin(x)}{2}\right) \quad \text{and} \quad g(x) = 2 \cos(x).$$

We take $D = (-\pi/2, \pi/2)$ and set $\psi(x) = 0$. Then we have the solution $u(x) = \cos(x)$. We evaluate numerically $u(0) = 1$.

We show results for the naive approach (Algorithm 1 with updates (23)) compared with the Algorithms 5 and 6. We have chosen sample sizes $N = 10^6$ and $N = 4 \cdot 10^6$. We show the approximate solutions and absolute errors. Confidence intervals $\hat{\sigma}$ are much smaller than the symbols used in the plot.

Solutions $\hat{u}(0)$ vs. stepsize h on top and error $|\hat{u}(0) - u(0)|$ vs. h on bottom.

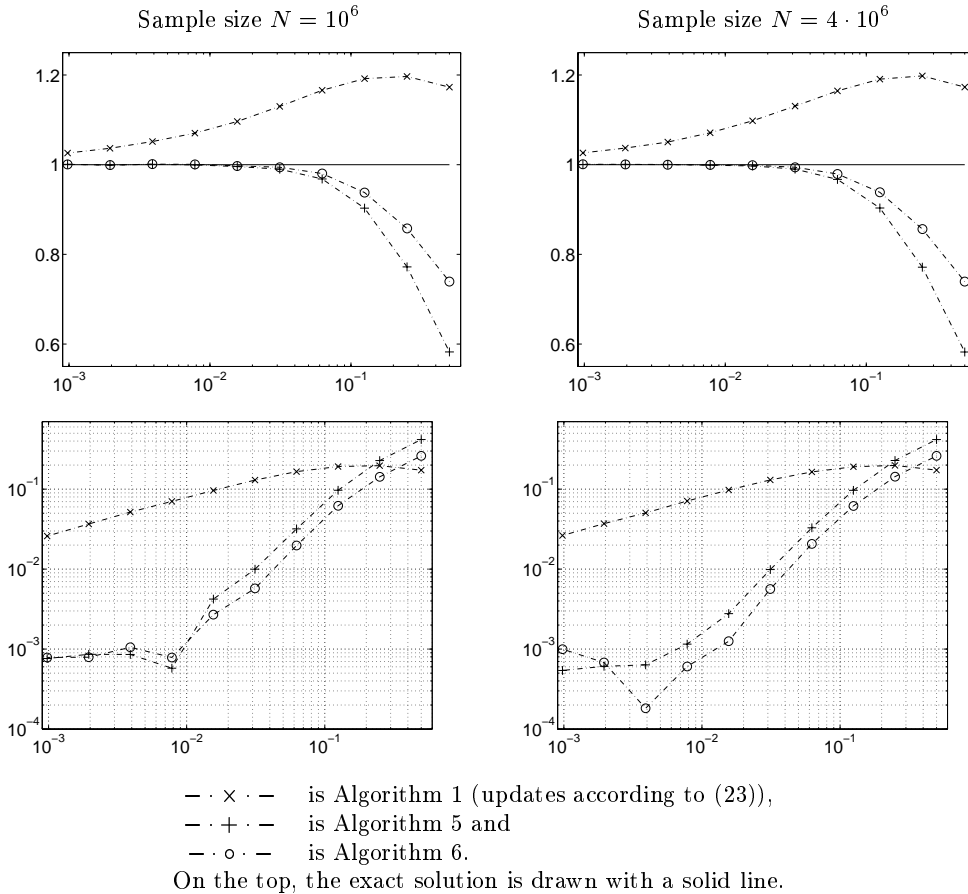


Figure 5: An exit test leads to convergence of at least weak order $\mathcal{O}(h)$ also in the case of general elliptic operators with connected general diffusions $dX = b(X) dt + \sigma(X) dW$. Generating \mathcal{H} improves results further at the same cost.

From Figure 5 we see, that the procedure works also for BVPs with general elliptic operators, as in (20). Both Algorithms 5 and 6 converge with a weak order of at least one whereas the simple approach converges only with order $\mathcal{O}(\sqrt{h})$. Further, Algorithm 6 improves the constant in the convergence order at the same computational cost.

5 Conclusions

We investigated the simplest numerical procedure for the approximation of SDEs: the Euler scheme. Although this scheme has been known, studied and used for a long time, its application in the presence of a boundary is still a field of active research. At the boundary, the path is killed, reflected or stopped. In each of these cases, the Euler scheme without any modification (see Algorithm 1) no longer converges with weak order one but only with order $\mathcal{O}(\sqrt{h})$. The problem arises because the simulated random walk is discrete (or linearly interpolated) and one has no information of the behaviour of the approximated path within the beginning and end of the step. In particular, the path might take an excursion across the boundary within a step which is missed by the discrete path. Simple yet effective modifications have been proposed in the literature, mainly for killed diffusions due to their interest in pricing barrier options.

Our interest is in stopped diffusions. Stopping the simulated process when it crosses the boundary gives an approximation to the first exit time – but to obtain again the lost weak order one

in convergence, improvements are needed. The adaptation of known procedures for killed diffusions to stopped ones worked encouragingly well. We showed how a simple exit test can avoid the loss in accuracy. Our numerical tests also revealed that testing for an excursion only across the *closest* boundary is permissible: the algorithms regain the first order in weak convergence (Figure 1). Already the obvious adaptation (Algorithm 2) showed good results (Figure 2). Nevertheless a simple modification based on a different interpretation of equation (9) led to Algorithm 3 which gave better results at the same computational cost (Figure 3 and Table 1). In the case of a pure Brownian motion we improved results further. There, we approximated the first hitting time of a bridge process across the boundary (Algorithm 4). Numerical experiments showed further decreasing errors. Finally, we generalized our ideas to more general diffusions which are connected with more general (elliptic) operators. A numerical test with non-constant drift and diffusion coefficients again showed satisfactory results.

We concentrated on the one dimensional situation. Expanding the ideas presented here to higher dimensions is under development. Additionally, the work of Janson and Lythe on exponential time stepping caught our interest. There, the main ideas to tackle the presence of a boundary are similar to the ones presented here – yet, the resulting formulae are much simpler.

Acknowledgements

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Appendix

From (15) it follows for $y < \beta < z$ that

$$\mathbb{P}_{y,h,z}[H_\beta(y) \in dt] = \frac{\tilde{\beta}}{\sqrt{2\pi h}} \frac{1}{\sqrt{\tilde{t}^3(1-\tilde{t})}} \exp\left(-\frac{1}{2h} \frac{(\tilde{\beta} - \tilde{t}z)^2}{\tilde{t}(1-\tilde{t})}\right) d\tilde{t}.$$

For simplicity of notation, we set $y = 0$ and $h = 1$ and show the calculations in this appendix only for the bridge pinned at $(0, 0)$ and $(1, z)$ with $0 < \beta < z$. The general bridge follows from these results in obvious manner. We have

$$\mathbb{P}_{0,1,z}[H_\beta(0) \in dt] = \frac{\beta}{\sqrt{2\pi}} \frac{1}{\sqrt{t^3(1-t)}} \exp\left(-\frac{1}{2} \frac{(\beta - tz)^2}{t(1-t)}\right) dt \quad (26)$$

and define $p(t)$ by $p(t)dt = \mathbb{P}_{0,1,z}[H_\beta(0) \in dt]$.

A Calculation of \hat{H}_{peak} (see (16))

To calculate $\arg \max_{0 < t < 1} p(t)$ define $u = u(t)$, $v = v(t)$, $w = w(t)$ as

$$p(t) = \frac{\beta}{\sqrt{2\pi}} \underbrace{\frac{1}{t\sqrt{t(1-t)}}}_{u(t)} e^{-\frac{1}{2} \frac{(\beta - tz)^2}{t(1-t)}} =: \frac{\beta}{\sqrt{2\pi}} u(t) e^{-\frac{1}{2} \frac{v(t)}{w(t)}}$$

(see (26)). Then, solving $dp(t)/dt = 0$ for $t \in (0, 1)$ reduces to solve $2u'w^2 - u(v'w - vw') = 0$ which shows to be equivalent to find the roots of the cubic polynomial $t^3 + lt^2 + mt + n = 0$ with

$$l = \frac{z^2 - 7 - 2\beta z}{4}, \quad m = \frac{3 + 2\beta^2}{4} \quad \text{and} \quad n = -\frac{\beta^2}{4}. \quad (27)$$

Introducing

$$q = \frac{2l^3}{54} - \frac{lm}{6} + \frac{n}{2}, \quad p = \frac{m}{3} - \frac{l^2}{9}, \quad D = p^3 + q^2 \quad \text{and} \quad P = \text{sgn}(q)\sqrt{|p|}$$

the real valued roots are given as $t_i = s_i - l/3$ where

$$\left. \begin{aligned} s_1 &= -2P \cos(\delta) \\ s_{2,3} &= 2P \cos(\delta \pm \frac{\pi}{3}) \end{aligned} \right\} \quad \text{with} \quad \delta = \frac{1}{3} \arccos(q/P^3) \quad \text{if} \quad p < 0 \quad \text{and} \quad D \leq 0,$$

$$s_1 = -2P \cosh(\delta) \quad \text{with} \quad \delta = \frac{1}{3} \text{Arcosh}(q/P^3) \quad \text{if} \quad p < 0 \quad \text{and} \quad D > 0,$$

$$s_1 = -2P \sinh(\delta) \quad \text{with} \quad \delta = \frac{1}{3} \text{Arsinh}(q/P^3) \quad \text{if} \quad p > 0.$$

For the general bridge pinned at $(0, y)$ and (h, z) we need the roots of the same polynomial as above where now (compare with (27))

$$l = \frac{(z-y)^2 - 7h - 2(\beta-y)(z-y)}{4}, \quad m = h \frac{3h + 2(\beta-y)^2}{4} \quad \text{and} \quad n = -h^2 \frac{(\beta-y)^2}{4}.$$

The formulas used in this appendix can be found in any standard handbook of mathematical formulae, for example [AS64, BS91].

B Proof of Lemma 1

To show $\mathbb{E}_{0,1,z}[H_\beta(0)] = C\beta$, we calculate the expectation explicitly. With (26) we have

$$\begin{aligned}\mathbb{E}_{0,1,z}[H_\beta(0)] &= \frac{\beta}{\sqrt{2\pi}} \int_0^1 \exp\left(-\frac{1}{2} \frac{(\beta - tz)^2}{t(1-t)}\right) \frac{dt}{\sqrt{t(1-t)}} \\ &= \frac{\beta}{\sqrt{2\pi}} \int_0^1 \exp\left(-\frac{z^2}{2} \frac{(\xi - t)^2}{t(1-t)}\right) \frac{dt}{\sqrt{t(1-t)}}\end{aligned}$$

where $\xi = \beta/z$. Introduce the transformation

$$x = \frac{t}{1-t} \quad \text{with} \quad \frac{dt}{\sqrt{t(1-t)}} = \frac{dx}{\sqrt{x(1+x)}}.$$

Let $\eta = 1 - \xi$, then

$$\frac{(\xi - t)^2}{t(1-t)} = \frac{(\xi - \eta x)^2}{x}.$$

With

$$p = \frac{z^2\eta^2}{2} = \frac{(z - \beta)^2}{2} \quad \text{and} \quad q = \frac{z^2\xi^2}{2} = \frac{\beta^2}{2}$$

we have

$$\mathbb{E}_{0,1,z}[H_\beta(0)] = \frac{\beta}{\sqrt{2\pi}} e^{z^2\xi\eta} \int_0^\infty \frac{e^{-px - \frac{q}{x}}}{\sqrt{x(1+x)}} dx.$$

We calculate the reminding integral

$$I = \int_0^\infty \frac{e^{-px - \frac{q}{x}}}{\sqrt{x}} \frac{1}{1+x} dx = \int_0^\infty \frac{e^{-px - \frac{q}{x}}}{\sqrt{x}} \int_0^\infty e^{-s(1+x)} ds dx.$$

Changing order of integration and using [PBM86, (2.3.16.3.), p.344]

$$\int_0^\infty e^{-(p+s)x - \frac{q}{x}} \frac{dx}{\sqrt{x}} = \sqrt{\frac{\pi}{p+s}} e^{-2\sqrt{(p+s)q}}$$

we have with $t = p + s$

$$I = \sqrt{\pi} e^p \int_p^\infty e^{-t} e^{-2\sqrt{qt}} \frac{dt}{\sqrt{t}}.$$

The obvious transformation $u^2 = t$ with $dt/\sqrt{t} = 2du$ yields after completing the square in the exponent

$$I = 2\sqrt{\pi} e^{p+q} \int_{\sqrt{p}}^\infty e^{-(u+\sqrt{q})^2} du = 2\sqrt{\pi} e^{p+q} \int_{\sqrt{p}+\sqrt{q}}^\infty e^{-v^2} dv = \pi e^{p+q} \operatorname{erfc}(\sqrt{p} + \sqrt{q})$$

where [AS64, (7.1.2), p.297]

$$\operatorname{erfc}(\zeta) = \frac{2}{\sqrt{\pi}} \int_\zeta^\infty e^{-v^2} dv = 1 - \operatorname{erf}(\zeta) = 1 - \frac{2}{\sqrt{\pi}} \int_0^\zeta e^{-v^2} dv.$$

Noting $z^2\xi\eta = \beta(z - \beta)$ and $\sqrt{p} + \sqrt{q} = z/\sqrt{2}$ we get finally

$$\mathbb{E}_{0,1,z}[H_\beta(0)] = \underbrace{\sqrt{\frac{\pi}{2}} e^{\frac{z^2}{2}} \operatorname{erfc}\left(\frac{z}{\sqrt{2}}\right)}_C \cdot \beta$$

which proofs Lemma 1 for $y = 0$ and $h = 1$.

For the bridge pinned at $(0, y)$ and (h, z) we find analogously for $y < \beta < z$

$$\mathbb{E}_{y,h,z}[H_\beta(y)] = \underbrace{\sqrt{\frac{h\pi}{2}} e^{\frac{(z-y)^2}{2h}} \operatorname{erfc}\left(\frac{z-y}{\sqrt{2h}}\right)}_C \cdot (\beta - y).$$

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