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Green's Functions by Monte Carlo

David White and Andrew Stuart

Abstract We describe a new numerical technique to estimate Green's functions of elliptic differential operators on bounded open sets. The algorithm utilizes SPDE based function space sampling techniques in conjunction with Metropolis-Hastings MCMC. The key idea is that neither the proposal nor the acceptance probability require the evaluation of a Dirac measure. The method allows Green's functions to be estimated via ergodic averaging. Numerical examples in both 1D and 2D, with second and fourth order elliptic PDE's, are presented to validate this methodology.

1 Introduction

Green's functions play a central role in many areas of mathematics and statistics: they provide fundamental solutions used as the basic building block to construct solutions of inhomogeneous PDEs; they act as the representers for reproducing kernel Hilbert spaces; and the covariance function of a Gaussian random field may be viewed as the Green's function for the precision operator.

This article describes a new numerical technique to estimate Green's functions of elliptic differential operators on bounded open sets. The algorithm utilizes SPDE based function space sampling techniques [3] in conjunction with Metropolis-Hastings MCMC [7]. The key idea is that neither the proposal nor the acceptance probability require the evaluation of a Dirac measure. The method estimates Green's functions via an ergodic average of sampled functions. The basic framework is that probability measures defined on a Hilbert space [4] are sampled using techniques designed specifically for this infinite dimensional setting.

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In Section 2 it is shown that a Gaussian measure on function space can be constructed with mean corresponding to the desired Green's function. The algorithm samples functions from this measure and the sample mean provides a good estimate of the Green's function of interest.

This idea is validated numerically by examples with known analytic solutions in Section 3. Green's functions of second and fourth order elliptic operators in both 1D and 2D are presented in this section.

The concept presented here is independent of the particular methodology used for sampling function space. Section 4 considers an alternative proposal for a function space MCMC sampling method and demonstrates the algorithm in this context via one of the numerical examples shown in Section 3.

2 Function Space Sampling and Algorithm Description

Sampling from a measure on function space is central to this algorithm. It is shown below that if the measure and function space sampling algorithm are constructed appropriately, then the ergodic average of suitably sampled functions converges to a Green's function of choice.

We begin by defining a probability measure π on a Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$. The measure π is constructed so that its mean is the desired Green's function on a bounded open set $D \subset \mathbb{R}^n$. Throughout this article the measure, π, has a Radon-Nikodym derivative with respect to a Gaussian measure π_0:

$$\frac{d\pi}{d\pi_0} \propto \exp(-\Theta(x)). \tag{1}$$

We chose a mean zero Gaussian reference measure $\pi_0 = \mathcal{N}(0, \mathcal{C})$ where $\mathcal{C}$ is a trace class, self adjoint, positive definite operator on $\mathcal{H}$ so that $\pi_0(\mathcal{H}) = 1$. For equation (1) we require that $\Theta : \mathcal{H} \to \mathbb{R}$ is π_0-measurable and integrable. The definition of π_0 may be combined with equation (1) to write the following informal expression for the target density as:

$$\pi(dx) \propto \exp\left(-\Theta(x) - \frac{1}{2}\langle x, \mathcal{C}^{-1}x\rangle\right) dx. \tag{2}$$

This expression has no rigorous status because there is no infinite dimensional equivalent of Lebesgue measure. However it conveys intuition about the measure which may be useful to the reader.

The algorithmic ideas presented in this paper apply to sampling general measures π of the form given by equation (1), in the case where π_0 is Gaussian [3]. However we now look at a particular choice of Θ arising in the application to the construction of Green's functions.

In order to obtain the Green's function of some elliptic differential operator $\mathcal{L}$ incorporating the boundary conditions through its domain, the covariance operator of the reference Gaussian measure is selected to be $\mathcal{C} = -\mathcal{L}^{-1}$. The function Hilbert space $\mathcal{H} = L^2(D)$ and Θ is chosen to be $\Theta(x) = \langle x, \delta_s \rangle$. Here δ_s is the Dirac delta function centered at $s \in D$.

By completing the square in equation (2) we deduce that $\pi \sim \mathcal{N}(\hat{x}, \mathcal{C})$ where $\hat{x} = -\mathcal{C}\delta_s$ or

$$\mathcal{L}\hat{x} = \delta_s. \tag{3}$$

Then π is absolutely continuous with respect to π_0 whenever $\hat{x} \in \operatorname{Im}\left(\mathcal{C}^{\frac{1}{2}}\right)$, by the Feldman-Hajek Theorem [4].

The measure π is invariant for the SPDE:

$$\frac{dx}{dt} = \mathcal{L}x - \delta_s + \sqrt{2}\frac{dw}{dt}. \tag{4}$$

Lemma 2.2 in [5] shows that this equation is well defined and ergodic.

Since equation (4) is invariant with respect to the target measure, π, the Green's function of interest may be obtained by time marching the SPDE and averaging the sampled functions to estimate $\hat{x}$. In practice, this requires direct evaluation of Dirac delta functions, which introduces further complications.

This difficulty may be circumvented as follows. Instead of equation (4) consider:

$$\frac{dx}{dt} = \mathcal{L}x + \sqrt{2}\frac{dw}{dt}. \tag{5}$$

Lemma 2.2 in [5] shows that equation (5) is π_0 invariant rather than π invariant. However equation (5) does not involve a Dirac delta function. If we use proposals based on discretising equation (5) then the Metropolis-Hastings accept/reject mechanism may be used to create a π invariant Markov chain.

Discretising the SPDE (5) using Crank-Nicolson gives equation:

$$\frac{y-x}{\Delta t} = \frac{\mathcal{L}x + \mathcal{L}y}{2} + \sqrt{\frac{2}{\Delta t}}\xi \tag{6}$$

where ξ represents a spatial white noise which is independent of the current state x. Re-arranging we obtain the proposal y given a current function x:

$$(2 - \Delta t\mathcal{L})\,y = (2 + \Delta t\mathcal{L})\,x + \sqrt{8\Delta t}\xi. \tag{7}$$

The acceptance probability for the proposal y given x is $\alpha(x, y)$ where:

$$\alpha(x, y) = \exp(0 \wedge R(x, y)), \tag{8a}$$

$$R(x, y) = \Theta(x) - \Theta(y) = x(s) - y(s). \tag{8b}$$

Notice that the acceptance probability only requires computation of the difference between the current and proposed functions at a single point. This is computationally inexpensive to evaluate and at no point in the algorithm do we need to evaluate a delta function.

This completes our explanation concerning the construction of the measure and the sampling algorithm. A more detailed explanation of function space sampling algorithms can be found in [3], for non-Gaussian measures, using SPDE which are invariant for π given by (1) see [5] and [6].

3 Examples and Numerics

This section numerically validates the above algorithm via three examples. The examples have known analytic solutions derived by techniques described in [1], [2] and [8].

Throughout this section we use the standard notation for Sobolev spaces H^s of functions with s square integrable derivatives, possibly incorporating periodic $\left(H^s_{\text{per}}\right)$ or Dirichlet $\left(H^s_0\right)$ boundary conditions.

Example 1. As a first example, we consider the elliptic differential operator $\mathcal{L} = \frac{d^2}{du^2}$ with Dirichlet boundary conditions:

$$\mathcal{L} = \frac{d^2}{du^2} \text{ on } (0,1) \tag{9a}$$

$$\text{with } D(\mathcal{L}) = \left\{x \in H^1_0(0,1) \cap H^2(0,1)\right\}. \tag{9b}$$

It may be shown theoretically that the Green's function for $\mathcal{L}$ is:

$$G(u,s) = \begin{cases} s(u-1) & \forall s \le u \\ u(s-1) & \forall s > u. \end{cases} \tag{10}$$

Figure 1 shows a numerical estimate of the Green's function (with $s = 0.3$) using 10^4 burn in steps and 10^5 actual steps of the MCMC method described in this article. A spatial discretisation of $\Delta u = 10^{-3}$ and time step of $\Delta t = 1$ were used here to generate these estimates. The initial function and the last sampled function are also displayed to demonstrate the stochastic origins of the estimate. The estimate appears to be approximately piecewise linear with a minimum at $u = 0.3$. These observed features are in agreement with the theory.

Example 2. The first example is generalised by introducing a second term into the differential operator. Equations (11a) and (11b) show the operator, interval and boundary conditions.

$$\mathcal{L} = \frac{d^2}{du^2} - k^2 \text{ on } (0,1) \tag{11a}$$

$$D(\mathcal{L}) = \left\{x \in H^1_0(0,1) \cap H^2(0,1)\right\} \tag{11b}$$

It may be shown theoretically that the Green's function for $\mathcal{L}$ is:

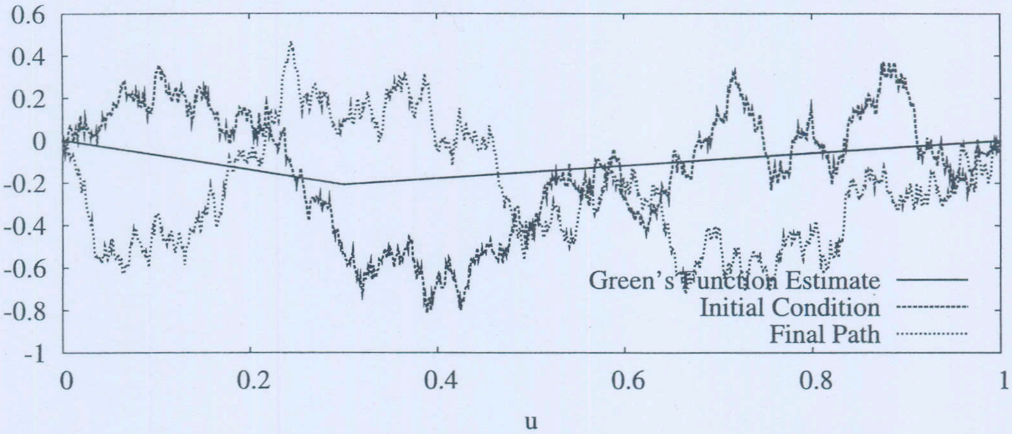


Fig. 1 Green's Function of $\mathcal{L} = \frac{d^2}{du^2}$ with $s = 0.3$.

$$G(u,s) = \begin{cases} \frac{e^{-k}}{2k}\frac{e^{ks}-e^{k(2-s)}}{e^k-e^{-k}}\left(e^{ku}-e^{-ku}\right) & \forall u \le s \\ \frac{e^{-k}}{2k}\frac{e^{ks}-e^{-ks}}{e^k-e^{-k}}\left(e^{ku}-e^{k(2-u)}\right) & \forall u > s. \end{cases} \tag{12}$$

The algorithm was tested using this problem with $\Delta u = 10^{-3}$, $\Delta t = 10^{-2}$ with a 10% burn in period. The initial condition function was chosen to be identically zero across [0, 1].

Figure 2 shows both (a) the numerical estimates of the Green's functions and (b) the L^2 normed error of these estimates for $k = 10$. (a) shows the Green's function estimate for 10^5 iterations and 10^8 iterations. The former has visible deviations from the correct solution and the latter is visually identical to the true solution. (b) shows the normed error of the algorithm's estimates for 10^5, 10^6, 10^7 and 10^8 samples. It is evident from these plots that the algorithm's output does converge to the correct solution.

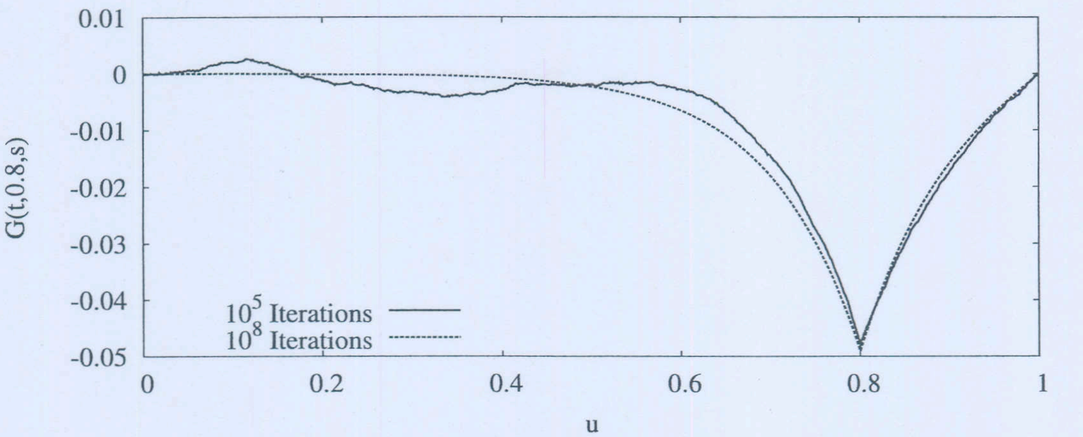
Example 3. We now consider a two-dimensional Green's function, arising from the biharmonic operator. The objective here is to test the algorithm on a higher dimensional problem. Define $\mathcal{L}$ by:

$$\mathcal{L} = -\Delta^2 = -\left(\frac{\partial^2}{\partial u_1^2} + \frac{\partial^2}{\partial u_2^2}\right)^2 \quad \text{on } E = (0,\ell_1)\times(0,\ell_2), \tag{13a}$$

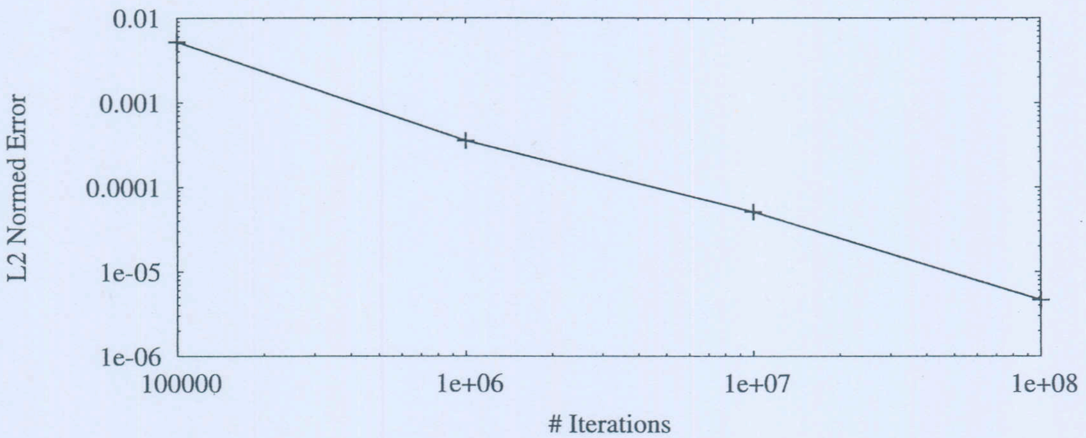
$$D(\mathcal{L}) = \left\{ x \in H^4_{\text{per}}(E) \,\middle|\, \int_E x\,du = 0 \right\}. \tag{13b}$$

The constraint shown in (13b) is required to uniquely define the Green's function. Without this, any constant may be added to a Green's function of $\mathcal{L}$ to obtain another valid Green's function.

Equation (14) shows the Green's function of this problem, calculated using Fourier series expansions:



(a) Numerical Green's Functions Estimates.



(b) Error in MCMC Estimates.

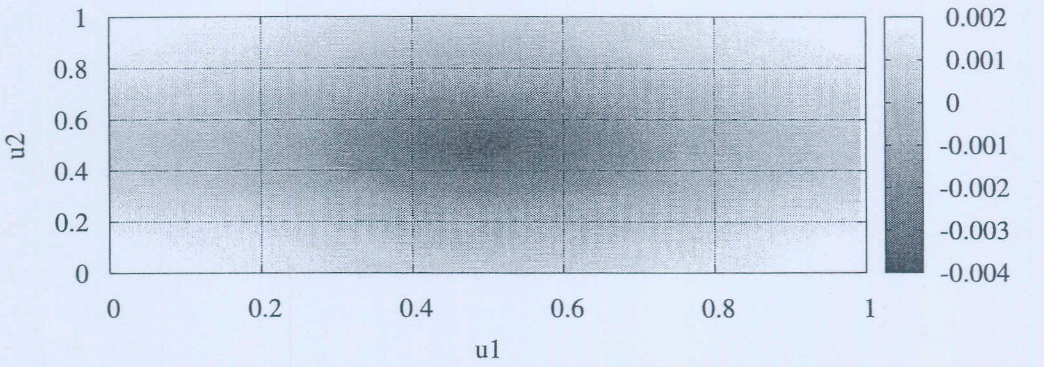
Fig. 2 Green's Function of $\mathcal{L} = \frac{d^2}{du^2} - 100$ with $s = 0.8$.

$$G\left(\underline{u}, \underline{s}\right) = -\frac{1}{16\pi^4 \ell_1 \ell_2} \sum_{(p,q)\in\mathbb{K}} \frac{\exp\left(\frac{2\pi i p(u_1 - s_1)}{\ell_1}\right)\exp\left(\frac{2\pi i q(u_2 - s_2)}{\ell_2}\right)}{\left(\frac{p^2}{\ell_1^2} + \frac{q^2}{\ell_2^2}\right)^2}. \tag{14}$$

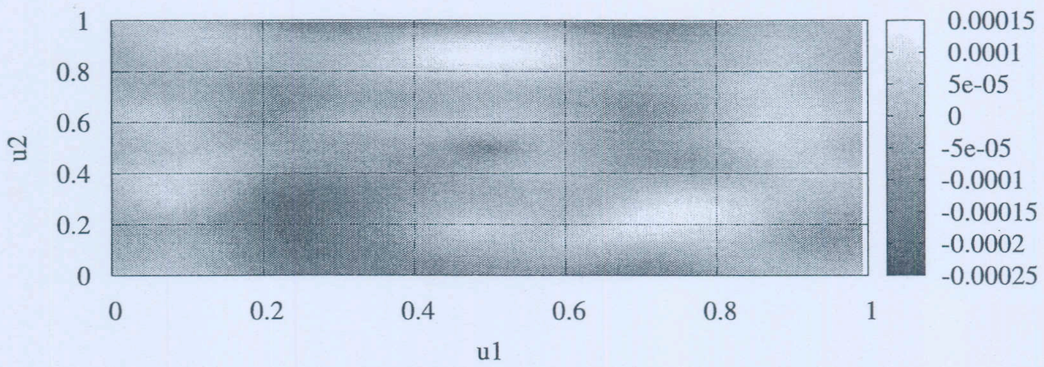
Here $\mathbb{K} = \mathbb{Z}^2 \setminus \{(0,0)\}$.

An FFT based approach was used to calculate proposals on $[0,1]^2$ using (7) and the accept/reject step was based on the function value at $s = \left(\frac{1}{2}, \frac{1}{2}\right)$. The discretisations and time steps used were $\Delta u_1 = \Delta u_2 = \frac{1}{128}$, $\Delta t = 1$ with 3.2×10^6 MCMC steps preceded by 10^5 burn in steps. The initial function was chosen to be identically zero on D.

Figure 3 shows (a) the resulting Green's function estimate and (b) the error estimate. It is clear from these plots that the algorithm functions correctly for this problem.



(a) Numerical Green's Functions Estimate.



(b) Error in MCMC Estimate.

Fig. 3 Green's Function of $\mathcal{L} = -\triangle^2$ with $s = (0.5, 0.5)$.

4 Other Related Proposals

A requirement of the algorithm presented in this paper is the invariance of the measure π to the SPDE stated in equation (4). However, this SPDE is not the only SPDE with this property. An alternative SPDE is (see [6], equation (2.14) and Theorem 3.6):

$$\frac{dx}{dt} = -x + \mathcal{C}\delta_s + \sqrt{2\mathcal{C}}\frac{dw}{dt}. \tag{15}$$

As above, $\mathcal{C}$ is the covariance operator and δ_s is the Dirac delta measure with centre at s.

The general definition of the square root of the self-adjoint operator $\mathcal{C}$ is, of course, through diagonalization in an orthonormal basis, as for matrices. Note however that if ξ is spatial white noise then $\sqrt{\mathcal{C}}\xi$ is simply a draw from the measure π_0; this may sometimes be achieved without constructing $\sqrt{\mathcal{C}}$ explicitly, for example if $\mathcal{C}$ is the covariance operator of Brownian bridge.

Similarly the following SPDE is π_0 invariant:

$$\frac{dx}{dt} = -x + \sqrt{2\mathcal{C}}\frac{dw}{dt}. \tag{16}$$

Similarly to the development in Section 2, this equation may be discretised and used to generate proposals for a Metropolis-Hastings Markov chain. The Crank-Nicolson discretisation gives:

$$\frac{y-x}{\Delta t} = -\frac{x+y}{2} + \sqrt{\frac{2\mathcal{C}}{\Delta t}}\xi \tag{17}$$

which re-arranges into:

$$y = \frac{2-\Delta t}{2+\Delta t}x + \frac{\sqrt{8\Delta t\mathcal{C}}}{2+\Delta t}\xi. \tag{18}$$

The re-arrangement has a special form, the proposal, y, is a linear combination of the current solution x and $\sqrt{\mathcal{C}}\xi$ where ξ is spatial white noise independent of x. In particular, $\sqrt{\mathcal{C}}\xi$ may be drawn directly from π_0. Also notice that:

$$\left(\frac{2-\Delta t}{2+\Delta t}\right)^2 + \frac{8\Delta t}{(2+\Delta t)^2} = 1. \tag{19}$$

This ensures that y is drawn from a measure which is absolutely continuous with respect to the Gaussian reference measure π_0. The acceptance probability for this proposal is again that shown in equations (8a) and (8b), (Theorem 4.1 in [3]).

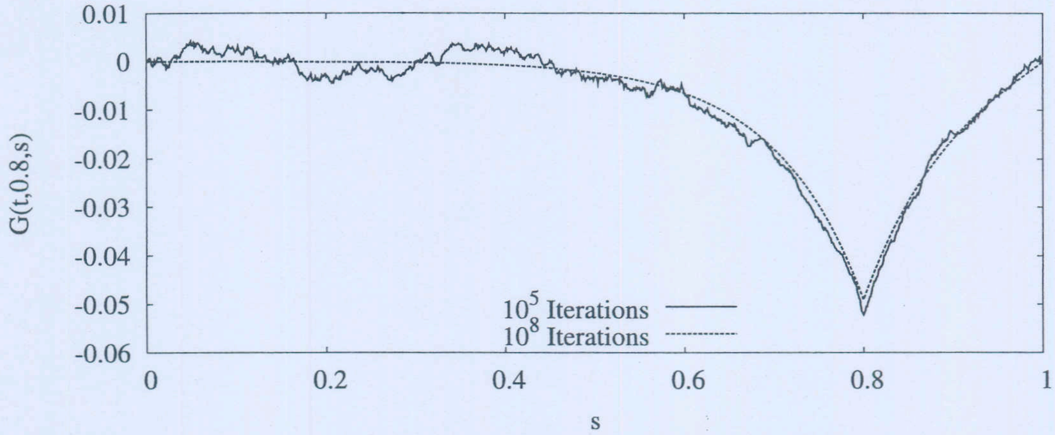
In one dimension, for the operator $\mathcal{L}$ given in Examples 1 and 2, $\sqrt{\mathcal{C}}\xi$ is Brownian bridge measure and draws from it can be made from linear combinations of Brownian motion.

The algorithm was tested using this problem with $\Delta u = 10^{-3}$, $\Delta t = 0.5$ with a 10% burn in period. The initial condition function was chosen to be identically zero across [0, 1].

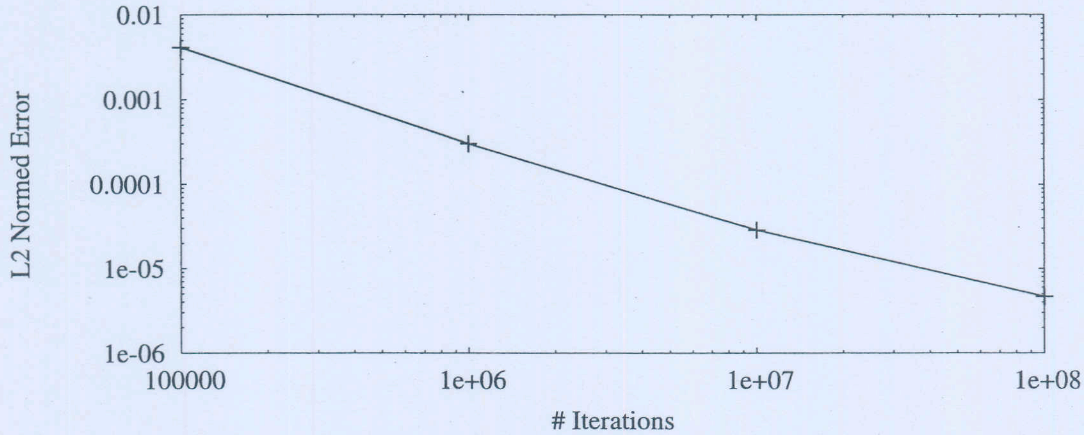
Figure 4 (a) shows estimates of the Green's function problem described in Example 2 and (b) shows the corresponding error norms produced using this alternate proposal. It is clear from these plots that the algorithm converges for this new proposal. This result is particularly interesting in view of the fact that the basic building block is simulation of Brownian motions (and hence Brownian bridges) and no inversion of $\mathcal{L}$ or $\mathcal{L}^{\frac{1}{2}}$ was required to generate this estimate.

5 Conclusions and Further Work

In this article we have introduced a new Metropolis-Hastings based approach to calculating Green's functions of elliptic operators on bounded open sets. It was shown that if the target measure is constructed on a function space in a particular way, the



(a) Numerical Green's Function Estimates.



(b) Error in MCMC Estimates.

Fig. 4 Green's Function of $\mathcal{L} = \frac{d^2}{du^2} - 100$ with $s = 0.8$ using the alternate SPDE proposal of Section 4.

ergodic average of the sampled functions converges to the Green's function of an elliptic differential operator.

The method was validated via three numerical examples, for which the Green's function was known analytically.

In addition to the work presented in this article, it has been observed that this algorithm is trivially parallelisable. Existing direct PDE based methods for calculating Green's functions are serial by necessity. So this potential for parallelism places a considerable advantage over existing methods. This work is on going and more details will appear in [9].

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