

A Sampling Method for Determining the Lowest Eigenvalue and the Principal Eigenfunction of Schrödinger's Equation¹

By M. D. Donsker and M. Kac

This is a preliminary report on a sampling method for finding the lowest eigenvalue and the corresponding eigenfunction of Schrödinger's equation. The theory underlying the procedure is explained and two cases treated numerically. Although the initial results are encouraging, more experimentation will be needed to fully test the practicality of the method.

I. Introduction

Certain problems leading to complicated partial or integro-differential equations have recently been approached and some actually solved by utilizing various probability techniques and sampling methods. Collectively these methods have become known as the "Monte Carlo" method.

The problems to which Monte Carlo techniques have been applied seem to be divided into two types. Typical of the first type is the problem of neutrons diffusing in material media in which the particles are subjected not only to certain deterministic influences but to random influences as well. In such a problem, the Monte Carlo approach consists in permitting a "particle" to play a game of chance, the rules of the game being such that the actual deterministic and random features of the physical process are step by step exactly imitated by the game. By considering very large numbers of particles, one can answer such questions as the distribution of the particles at the end of a certain period of time, the number of particles to escape through a shield of specified thickness, etc. One important characteristic of the preceding approach is that the functional equation describing the diffusion process is bypassed completely, the probability model used being derived from the process itself.

A more sophisticated application of Monte

Carlo methods is to the problem of finding a probability model or game whose solution is related to the solution of a partial differential equation, or, as in the present paper, to determine the least eigenvalue of a differential operator by means of a sampling process. As an example of how the latter problem might be attacked, we quote from a paper of Metropolis and Ulam:²

"For example, as suggested by Fermi, the time independent Schrödinger equation

$$\Delta\phi(x,y,z) = (\lambda - V)\phi(x,y,z),$$

could be studied as follows. Reintroduce time dependence by considering

$$u(x,y,z,t) = \phi(x,y,z)e^{-\lambda t};$$

then, u will obey the equation

$$\frac{\partial u}{\partial t} = \Delta u - Vu.$$

This last equation can be interpreted, however, as describing the behavior of a system of particles each of which performs a random walk, i. e., diffuses isotropically and at the same time is subject to multiplication, which is determined by the value of the point function V . If the solution of the latter equation corresponds to a spatial

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² N. Metropolis and S. Ulam, The Monte Carlo method, J. Am. Stat. Assn. 44, 247, pp. 335 to 341 (Sept. 1949).

mode multiplying exponentially in time, the examination of the spatial part will give the desired $\phi(x, y, z)$ —corresponding to the lowest ‘eigenvalue’ λ .³

The main purpose of the present paper is to present an alternative method for finding the lowest eigenvalue and corresponding eigenfunction of Schrödinger’s equation. The chief difference between the two approaches is that ours involves only a random walk eliminating entirely the multiplicative process. This alteration in the model seems to simplify the numerical aspects of the problem, especially if punched card equipment is to be used. Apart from the possible numerical simplification, the method is based on a mathematical theory that in itself is of some interest.

II. Mathematical Theory

Let X_1, X_2, X_3, \dots be independent identically distributed random variables each having mean 0 and standard deviation 1 and let $S_k = X_1 + X_2 + \dots + X_k$. Under certain general assumptions on $V(x)$, the most severe of which is that $V(x)$ be nonnegative, it can be shown⁴ that the limiting distribution function $\sigma(\alpha, t)$ of the random variable

$$\frac{1}{n} \sum_{k < nt} V\left(\frac{S_k}{\sqrt{n}}\right) \quad (1)$$

is such that

$$\int_0^\infty \int_0^\infty e^{-\alpha-s t} d_\alpha \sigma(\alpha, t) dt = \int_{-\infty}^\infty \psi(x) dx, \quad (2)$$

where $\psi(x)$ is the fundamental solution of the differential equation

$$\frac{1}{2} \frac{d^2 \psi}{dx^2} - (s + V(x)) \psi = 0, \quad (3)$$

subject to the conditions

$$\begin{aligned} \psi(x) &\rightarrow 0 & x &\rightarrow \pm \infty \\ |\psi'(x)| &< M & x &\neq 0 \\ \psi'(+0) - \psi'(-0) &= -2. \end{aligned}$$

The fundamental solution $\psi(x)$ of (3) is expressible in terms of the normalized eigenfunction

$\{\psi_j(x)\}$ and eigenvalues λ_j of the one-dimensional Schrödinger eigenvalue problem⁵

$$\frac{1}{2} \frac{d^2 \psi}{dx^2} - V(x) \psi(x) = -\lambda \psi \quad \lambda > 0 \quad (4)$$

as

$$\psi(x) = \sum_j \frac{\psi_j(0) \psi_j(x)}{s + \lambda_j}. \quad (5)$$

Thus from (5 and 2)

$$\begin{aligned} \int_{-\infty}^\infty \psi(x) dx &= \int_0^\infty \int_0^\infty e^{-\alpha-s t} d_\alpha \sigma(\alpha, t) dt \\ &= \sum_j \frac{\psi_j(0) \int_{-\infty}^\infty \psi_j(x) dx}{s + \lambda_j}. \end{aligned} \quad (6)$$

Inverting (6) with respect to s we get,

$$\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t) = \sum_j e^{-\lambda_j t} \psi_j(0) \int_{-\infty}^\infty \psi_j(x) dx, \quad (7)$$

and therefore we obtain the expression for λ_1 ,

$$\lambda_1 = \lim_{t \rightarrow \infty} -\frac{1}{t} \log \int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t). \quad (8)$$

If in (7) we neglect all terms in the expansion but the first, we obtain

$$\log \int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t) \sim \log \left\{ \psi_1(0) \int_{-\infty}^\infty \psi_1(x) dx \right\} - \lambda_1 t,$$

or

$$\lambda_1 \sim \frac{\log \left\{ \psi_1(0) \int_{-\infty}^\infty \psi_1(x) dx \right\}}{t} - \frac{1}{t} \log \int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t). \quad (9)$$

Thus, if, by choosing a finite t , we attempt to calculate λ_1 from (8), we have two sources of error. The first, usually a small source of error, is from the exponentials neglected in the expansion (7). The second, and more important, is from neglecting the term $(1/t) \log \left\{ \psi_1(0) \int_{-\infty}^\infty \psi_1(x) dx \right\}$. This latter source of error is especially significant, since, as will be apparent shortly, it is impractical from other points of view to take t very large. All of this difficulty may be obviated by considering (7) for two distinct values of t , say t_1 and t_2 , then, if

³ We have since learned that Dr. G. W. King has made similar calculations using a closely related method.

⁴ M. Kac, On distributions of certain Wiener functionals, Trans. Am. Math. Soc. **65**, 1 to 13 (1949).

⁵ From here on all the steps are formal. In all cases of physical interest they can be justified rigorously.

we neglect the exponentials after the first as before, we get on dividing

$$\lambda_1 \sim \frac{1}{t_2 - t_1} \log \frac{\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t_1)}{\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t_2)}. \quad (10)$$

The Monte Carlo process consists in the calculation of $\sigma(\alpha, t_1)$ and $\sigma(\alpha, t_2)$ by a sampling process.

If instead of $\sigma(\alpha, t)$ we consider the limiting distribution $\sigma_\xi(\alpha, t)$ of the random variable

$$\frac{1}{n} \sum_{k \leq nt} V\left(\xi + \frac{S_k}{\sqrt{n}}\right), \quad (11)$$

then $\sigma_\xi(\alpha, t)$ also satisfies (2 and 3), but now the condition $\psi'(+0) - \psi'(-0) = -2$ is replaced by $\psi'(\xi+) - \psi'(\xi-) = -2$. Therefore, repeating steps (4 to 7), we get

$$\int_0^\infty e^{-\alpha} d_\alpha \sigma_\xi(\alpha, t) = \sum_j e^{-\lambda_j t} \psi_j(\xi) \int_{-\infty}^\infty \psi_j(x) dx. \quad (12)$$

Thus

$$\frac{\psi_1(\xi)}{\psi_1(0)} = \lim_{t \rightarrow \infty} \frac{\int_0^\infty e^{-\alpha} d_\alpha \sigma_\xi(\alpha, t)}{\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t)}, \quad (13)$$

so that we are also able to calculate the principal eigenfunction.

The extension of the preceding method to multi-dimensional Schrödinger equations is immediate. It is in these cases that the method will probably prove to be most useful since, unlike the standard variational procedures, the extension to several dimensions seems to cause comparatively little difficulty. For illustrative purposes we will consider Schrödinger's equation in three dimensions. Here we must consider three independent sequences

$$X_1, X_2, X_3, \dots,$$

$$Y_1, Y_2, Y_3, \dots,$$

$$Z_1, Z_2, Z_3, \dots,$$

of independent identically distributed random variables each having mean 0 and standard deviation 1. Let $S_{xk} = X_1 + X_2 + \dots + X_k$, and S_{yk} , S_{zk} have the obvious meanings. We consider the limiting distributions $\sigma(\alpha, t)$ and $\sigma(\alpha, \xi, \eta, \zeta, t)$ of the random variables

$$\frac{1}{n} \sum_{k \leq nt} V\left(\frac{S_{xk}}{\sqrt{n}}, \frac{S_{yk}}{\sqrt{n}}, \frac{S_{zk}}{\sqrt{n}}\right),$$

and

$$\frac{1}{n} \sum_{k \leq nt} V\left(\xi + \frac{S_{xk}}{\sqrt{n}}, \eta + \frac{S_{yk}}{\sqrt{n}}, \zeta + \frac{S_{zk}}{\sqrt{n}}\right),$$

respectively.

In exactly the same way as in the one dimensional case, we arrive at

$$\lambda_1 \sim \frac{1}{t_2 - t_1} \log \frac{\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t_1)}{\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t_2)},$$

and

$$\frac{\psi_1(\xi, \eta, \zeta)}{\psi_1(0, 0, 0)} = \lim_{t \rightarrow \infty} \frac{\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, \xi, \eta, \zeta, t)}{\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t)}.$$

So far, the theory was carried out under the assumption that the potential function V was nonnegative. In most cases of physical interest this is not so. For the hydrogen atom, for instance

$$V(x, y, z) = -\frac{\text{const.}}{\sqrt{x^2 + y^2 + z^2}}.$$

However, the modification is easy, although we have not as yet cleared up all the points of mathematical rigor.

The formula for the lowest eigenvalue now becomes

$$\lambda_1 \sim \frac{1}{t_2 - t_1} \log \frac{\int_{-\infty}^0 e^{-\alpha} d_\alpha \sigma(\alpha, t_1)}{\int_{-\infty}^0 e^{-\alpha} d_\alpha \sigma(\alpha, t_2)},$$

and a corresponding modification needs to be made in the formula for the principal eigenfunction. We have not yet tested numerically any case with a negative potential function, but we hope to be able to report on this in the near future.

III. Numerical Examples and Discussion

The Monte Carlo procedure used here consists in the calculation of the distribution function $\sigma(\alpha, t)$ by a sampling process; the principal eigenvalue is then calculated from (10). For the purposes of numerical illustration we consider two examples, $V(x) = x^2$ and $V(x) = |x|$. In both of

these cases the eigenvalues are known, and hence we have a check on the accuracy of our procedure. In order to calculate $\sigma(\alpha, t)$, say when $V(x) = x^2$, we see from (1) that we must consider the limiting distribution as $n \rightarrow \infty$ of

$$\frac{1}{n^2} \sum_{k \leq nt} S_k^2. \quad (14)$$

This means from our point of view that we must (a) choose a distribution for the X 's, (b) choose a sufficiently large n , (c) select an appropriate t , (4) calculate for nt X 's the normalized sum (14), (5) repeat (4) many times, so that the empirical distribution may be obtained from these many samples.

Although, under the conditions mentioned previously, the distribution function $\sigma(\alpha, t)$ is independent of the distribution of the X 's, the actual numerical calculation of $\sigma(\alpha, t)$ is expedited by choosing the distribution of the X 's to be the Bernoulli distribution, i. e.,

$$P(X=1) = P(X=-1) = \frac{1}{2}.$$

The sequence of random variables X_1, X_2, X_3, \dots is then a sequence of $+1$'s and -1 's, such as might be obtained in coin tossing. This is conveniently and rapidly achieved on a calculating machine by considering sequences of random digits, counting even digits $+1$ and odd digits -1 .

The value of n to be used must be large enough so that the empirical distribution function calculated is close to the theoretical limiting distribution function $\sigma(\alpha, t)$. From (10) we see that the two values of t, t_1 , and t_2 , to be used in the calculation of λ must be large enough so that the exponential terms neglected are sufficiently small. However, since the sample size is nt , the desire to make both n and t large must be tempered by practical considerations. The number of samples to be used must be large enough so that the empirical distribution adequately represents $\sigma(\alpha, t)$. Before discussing these points in more detail we consider an actual numerical computation. The following data for $V(x) = x^2$ and $V(x) = |x|$ were calculated from a certain set of random digits⁶ on the IBM Electronic Calculating Punch, Type 604. For both x^2 and $|x|$ n was selected to be 400,

⁶ This set of random digits was prepared by the RAND Corporation, Santa Monica, Calif.

$t_1 = 5, t_2 = 3.75$, and 100 samples were used. In table 1 is tabulated

$$A_1 = \frac{1}{8000} \sum_{k=1}^{1500} |S_k|, \quad A_2 = \frac{1}{8000} \sum_{k=1}^{2000} |S_k|,$$

$$B_1 = \frac{1}{160000} \sum_{k=1}^{1500} S_k^2, \quad B_2 = \frac{1}{160000} \sum_{k=1}^{2000} S_k^2.$$

Since each RAND random number card contains 50 random digits, and 2,000 digits are needed to form one sample, a set of 4,000 RAND cards was sufficient for this experiment. It takes 20 minutes on the IBM 604 to calculate A_1 and A_2 for one sample (similarly for B_1 and B_2), so that it takes approximately 35 hours to secure the following data.

TABLE 1. *Experimental data for lowest eigenvalue*

	A_1	A_2	B_1	B_2
1	1.332	2.101	0.738	1.290
2	3.808	5.707	5.295	8.502
3	2.795	5.545	3.460	9.610
4	8.723	13.917	30.722	52.616
5	4.169	4.766	6.123	6.602
6	1.195	2.136	.598	1.453
7	6.674	12.112	15.258	39.058
8	4.103	5.242	5.826	7.004
9	5.751	8.840	10.440	18.143
10	4.250	4.981	6.069	6.679
11	2.909	5.643	3.844	10.044
12	2.834	3.416	3.602	4.097
13	1.888	2.194	1.595	1.700
14	2.022	2.337	1.510	1.638
15	1.680	3.908	1.184	5.289
16	7.700	12.712	24.769	44.936
17	3.228	4.973	3.563	6.145
18	1.844	2.654	1.523	2.183
19	2.376	5.275	2.017	8.854
20	4.533	5.640	6.380	7.616
21	4.209	7.543	7.735	16.703
22	3.847	5.590	6.666	9.204
23	5.206	6.314	9.148	10.600
24	1.962	2.698	1.859	2.923
25	3.523	4.807	5.084	6.482
26	3.605	5.397	5.014	7.680
27	9.168	13.692	27.973	44.461
28	5.625	7.898	11.528	16.010
29	3.215	4.152	3.362	4.170
30	3.293	3.972	4.136	4.677
31	2.710	3.683	3.006	4.025
32	3.638	7.386	6.114	17.413
33	7.928	11.567	25.084	36.001
34	3.475	3.846	4.396	4.550
35	1.958	2.594	1.457	1.948
36	5.356	7.216	8.888	11.781
37	3.297	6.395	3.800	11.555
38	1.883	2.682	1.387	1.995
39	4.849	10.020	8.396	30.233
40	2.282	3.067	2.258	2.882

TABLE 1. *Experimental data for lowest eigenvalue—Con.*

	A_1	A_2	B_1	B_2
41	4.253	6.957	6.744	13.502
42	7.559	8.834	17.143	18.702
43	1.122	2.587	.500	2.634
44	1.433	3.602	.869	4.855
45	2.984	3.477	2.851	3.161
46	1.677	3.158	1.025	3.341
47	5.145	9.697	11.941	28.826
48	4.982	9.140	9.201	23.092
49	1.675	2.152	1.129	1.472
50	1.580	3.375	1.147	3.807
51	2.606	3.621	2.254	3.247
52	4.303	5.883	7.987	10.104
53	7.553	12.092	19.632	36.427
54	3.138	5.703	3.968	9.325
55	3.343	4.327	4.264	5.380
56	1.423	2.315	0.770	1.533
57	7.996	11.458	21.405	31.585
58	1.916	2.744	1.253	1.959
59	1.490	2.161	0.789	1.404
60	3.536	5.382	4.125	7.461
61	6.278	11.060	16.187	34.779
62	1.174	1.709	0.573	0.919
63	5.272	9.919	10.463	27.825
64	3.576	5.277	6.021	8.707
65	2.686	5.081	3.577	8.307
66	6.166	8.785	14.056	19.627
67	4.412	5.548	6.095	7.182
68	1.732	4.664	1.170	8.720
69	2.730	4.970	2.440	6.639
70	1.331	2.772	0.765	2.642
71	3.668	5.318	5.730	8.001
72	2.948	3.801	3.248	4.104
73	5.279	8.931	12.455	23.513
74	11.284	15.784	41.684	58.525
75	2.183	2.787	2.086	2.455
76	4.298	7.427	9.139	17.157
77	1.412	2.893	0.894	3.490
78	2.002	2.567	1.602	2.024
79	2.619	3.780	2.981	4.205
80	2.695	4.616	2.974	6.077
81	4.706	6.672	8.330	11.487
82	5.517	7.981	9.846	14.805
83	1.755	2.099	1.066	1.207
84	2.084	2.876	1.735	2.504
85	1.574	2.743	0.993	2.256
86	5.818	10.444	13.322	30.522
87	4.387	7.844	9.037	18.695
88	3.666	5.244	4.416	6.541
89	7.111	13.311	19.834	50.822
90	6.280	8.548	13.403	17.587
91	4.872	5.836	9.230	10.023
92	3.035	3.323	2.865	2.973
93	3.608	4.697	4.256	5.357
94	3.977	4.964	5.215	6.242
95	3.614	7.867	5.757	20.434
96	9.193	11.183	27.789	31.075
97	4.108	5.282	5.918	7.374
98	4.355	5.744	7.774	10.223
99	1.898	2.661	1.507	2.013
100	9.683	17.154	35.803	80.543

In order to calculate λ_1 from (10) we need the values of $\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t_1)$ and $\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t_2)$. Both of these integrals were calculated numerically from the data in table 1 by adding the exponentials of the entries in appropriate columns. For the case $V(x) = |x|$, the values of the integrals were obtained from $1/100 \sum_{i=1}^{100} e^{-A_{1i}}$ and $1/100 \sum_{j=1}^{100} e^{-A_{2j}}$ and for $V(x) = x^2$ from $1/100 \sum_{i=1}^{100} e^{-B_{1i}}$ and $1/100 \sum_{j=1}^{100} e^{-B_{2j}}$. In the case $V(x) = |x|$ the true lowest eigenvalue to two places is 0.81, and in the case $V(x) = x^2$ it is $\sqrt{2}/2 = 0.71$.

	First 50 samples	Second 50 samples	All 100 samples
$ x $	0.83	0.79	0.81
x^2	.80	.69	.75

An interesting feature of the data is that column B_2 , for example, may be thought of as arising from $n=2000, t=1; n=1000, t=2$, etc., as well as from $n=400, t=5$. The larger we take n , the closer will be the empirical distribution to $\sigma(\alpha, t)$. The value of $\int_0^\infty e^{-\alpha} d_\alpha \sigma(\alpha, t)$ in the case $t=1$, and $V(x) = x^2$ can be calculated exactly and, to three places, is 0.678. Calculating this integral from column B_2 with $n=2000, t=1$, we get 0.685.

Instead of using Bernoulli distributed variables, one might use other distributions. One definite advantage of Bernoulli distributed variables is that the computation utilizes only the crudest properties of the random digits, i. e., whether they are even or odd. One possible advantage for certain other distributions is that n might not have to be taken so large. In particular this should be true if we use Gaussian distributed variables. RAND Gaussian deviates were used in constructing table 2. Here we chose $t_1=3.75, t_2=5$ as before, but now $n=100$. This means samples of size 500 instead of 2000 and therefore a total machine computation time of 9 hours for 100 samples.

Envisaging the possibility of calculating the second eigenvalue, we considered the quantities

$$10^{-4} \sum_{k=1}^{375} (S_k + 5)^2 \text{ and } 10^{-4} \sum_{k=1}^{500} (S_k + 5)^2, \quad (15)$$

TABLE 2. Experimental data for second eigenvalue

	C_1	C_2		C_1	C_2
1	3.963	13.997	61	49.929	84.307
2	2.348*	2.721	62	3.095	6.220
3	1.889*	2.251	63	2.585*	3.867*
4	3.817*	4.372*	64	1.318*	1.906*
5	2.395	2.802*	65	2.241*	9.102*
6	12.467	27.683	66	9.737	12.185
7	1.068*	1.115*	67	9.738*	11.347*
8	0.578*	0.967*	68	4.604	5.589
9	1.504*	1.760	69	20.364	29.707
10	4.249	9.787	70	1.097*	1.895*
11	1.751*	3.316*	71	5.891	13.391
12	9.922	13.975	72	9.019*	12.815*
13	5.680	6.649	73	1.843	6.280
14	3.348	4.684	74	7.961	11.431
15	13.431	24.769	75	1.109	1.926
16	1.473*	2.615*	76	2.417*	3.037
17	45.262	74.304	77	2.402*	2.797*
18	1.157*	3.109	78	2.043*	4.214*
19	0.906*	3.644*	79	0.582*	0.752
20	4.601	12.641	80	2.429	4.381
21	8.356*	13.084*	81	8.584	13.054
22	0.308*	1.874*	82	2.793*	4.659*
23	2.111*	4.428*	83	1.557	5.023
24	2.035*	2.726	84	1.006*	1.677*
25	1.625*	3.898	85	5.327*	15.531*
26	1.879*	5.713	86	2.058	7.307
27	1.533	8.961	87	12.481	12.803*
28	1.769	2.319*	88	0.925*	2.403
29	1.906*	2.417*	89	15.519	19.879
30	7.522	7.979*	90	1.456*	4.009*
31	14.934	15.493*	91	5.244	10.047
32	4.282*	13.747*	92	2.497	2.931
33	1.356*	2.718	93	16.700	17.382
34	4.448	8.329	94	4.471*	8.156*
35	1.306*	2.112*	95	2.139*	2.580*
36	5.465*	12.396*	96	1.196*	2.273*
37	2.918	9.006	97	23.014	28.420
38	35.821	56.626	98	6.959*	7.022*
39	9.814*	11.707*	99	3.374*	8.651*
40	1.811	4.628	100	1.600*	2.250*
41	3.374	6.460	101	4.626*	7.794*
42	1.633	6.578	102	5.195*	10.215*
43	6.976	8.705	103	6.837*	12.160*
44	7.595	13.096	104	1.913	4.412*
45	2.336	2.862	105	2.276*	2.770
46	1.931*	2.579*	106	1.935*	3.983*
47	4.507*	8.294*	107	3.560	5.808
48	8.581*	11.301*	108	2.857*	7.384*
49	4.698*	8.220*	109	3.399*	4.484*
50	10.154	16.884	110	6.917*	27.107*
51	8.828	15.387	111	38.661	56.479
52	0.997*	1.604*	112	1.891	2.000*
53	8.582	12.838	113	8.506	9.646*
54	2.730*	3.249*	114	4.209	10.461
55	10.471	13.140	115	33.194	44.247
56	1.456*	1.845*	116	0.869*	1.289
57	8.230*	11.924*	117	3.946	15.204
58	5.515*	8.146*	118	1.680*	2.995*
59	2.202*	3.182*	119	8.178*	9.056
60	2.129*	9.650*	120	27.621	51.650

TABLE 2. Experimental data for second eigenvalue—Con.

	C_1	C_2		C_1	C_2
121	8.444*	15.836*	161	3.546	4.040*
122	13.254	16.467	162	1.238*	2.304*
123	1.755*	5.246*	163	0.975*	1.283
124	36.902	70.134	164	1.980	3.659*
125	7.567*	18.553*	165	14.620*	17.565*
126	14.725	38.551	166	2.378*	2.865
127	0.983*	2.572	167	2.279	6.279
128	24.529	31.660	168	10.846	13.754
129	2.042*	2.385*	169	1.341*	3.673*
130	3.587*	9.858*	170	1.861*	2.729*
131	1.335*	1.755	171	28.588*	53.358*
132	2.142*	3.801*	172	2.943	3.087*
133	16.361	27.759	173	1.694	2.568
134	8.193	9.301	174	1.729	2.516*
135	2.719*	5.141*	175	0.844*	1.449*
136	4.767*	12.737*	176	3.441*	5.380*
137	42.230	108.038	177	0.712	0.838*
138	41.236	78.423	178	1.222*	3.469*
139	8.243	9.911*	179	20.852*	42.263*
140	31.522	36.393	180	7.575*	16.552*
141	2.600	2.881*	181	2.042*	3.058
142	1.932	2.055*	182	6.797	7.343*
143	8.562	10.813	183	1.536	4.499
144	1.421*	3.652*	184	1.235	1.472*
145	2.669*	3.889*	185	3.541*	4.272
146	1.125*	2.071	186	5.394*	6.149*
147	3.439*	5.824*	187	18.589	28.787
148	1.269*	5.651	188	8.372	12.628
149	7.949	14.252	189	13.470*	23.775*
150	2.808*	4.434*	190	1.196*	2.851*
151	6.413	12.573	191	3.507	7.712
152	5.936*	10.432*	192	21.489	43.372
153	9.788	18.093	193	1.038*	1.109*
154	1.251	2.707	194	3.591*	3.864
155	34.799	63.494	195	2.295*	2.529*
156	0.841*	1.742*	196	1.044*	2.320
157	1.461*	1.615*	197	4.865*	6.759*
158	7.220	21.125	198	1.184	11.852
159	1.275*	2.359*	199	1.228*	1.969*
160	9.355	19.565	200	9.346*	22.204*

which correspond to taking $\xi=0.5$ in (11). This should not make any difference in the calculation of the lowest eigenvalue, and consequently table 2 can be utilized in the same way as table 1. It should however be borne in mind that columns C_1 and C_2 of table 2 represent experimental values of the quantities (18) with the S_k 's being sums of Gaussian deviates. Asterisks on the entries of table 2 indicate that S_{375} or S_{500} was negative. Although this information is unnecessary for the purpose of calculations of the lowest eigenvalue, it is used in the calculation of the next eigenvalue. How this can be done is explained briefly in section IV.

Using the data in table 2 and again (10) we computed the following approximations to λ_1 (actual value=0.71)

	First 50 samples	Second 50 samples	Third 50 samples	Fourth 50 samples	All 200 samples
λ_1	0.82	0.72	0.83	0.64	0.74

For both $V(x)=|x|$ and $V(x)=x^2$, all the eigenvalues are known so that in the two illustrative examples above it was easy to choose appropriate values for t_1 and t_2 . The proper value for n and the appropriate number of samples was determined experimentally. In general when all eigenvalues are unknown the following "rule of thumb" procedure seems to be feasible. Having first made a guess at an appropriate n and t , and a certain number of samples, compute λ_1 . Repeat the computation now for the same n , the same number of samples and successively larger t 's until the calculated values of λ_1 become stable to the desired number of places. If they do not become stable, the number of samples must be increased. Keeping two values of t , for which the calculated λ 's had the stable value, increase n and see if the calculated value of λ changes. If not, n is sufficiently large. If it does change, increase n until a new stability appears. This stable value is then the appropriate approximation to λ_1 . The mere fact that stability is observed means the number of samples is sufficiently large.

The Second Eigenvalue

If the principal eigenfunction is even, then it is possible to extend the theory of section II in such a way that the calculation of the second eigenvalue becomes feasible. Without going into any details we just state the pertinent result: Let

$$E_t^+(\xi) = \lim_{n \rightarrow \infty} E \left\{ e^{-\frac{1}{n} \sum_{k \leq nt} V\left(\xi + \frac{S_k}{\sqrt{n}}\right)} \mid S_{nt} > 0 \right\}, \quad (16)$$

and

$$E_t^-(\xi) = \lim_{n \rightarrow \infty} E \left\{ e^{-\frac{1}{n} \sum_{k \leq nt} V\left(\xi + \frac{S_k}{\sqrt{n}}\right)} \mid S_{nt} < 0 \right\}, \quad (17)$$

the mathematical expectations on the right hand sides being *conditional* expectations under the conditions $S_{nt} > 0$ and $S_{nt} < 0$, respectively.

We then have

$$\frac{1}{2} \left\{ E_t^+(\xi) - E_t^-(\xi) \right\} = \sum_{j=2}^{\infty} e^{-\lambda_j t} \psi_j(\xi) \int_{-\infty}^{\infty} \rho(x) \psi_j(x) dx, \quad (18)$$

where

$$\rho(x) = \begin{cases} +1, & x > 0 \\ -1, & x < 0. \end{cases}$$

If t_1 and t_2 are sufficiently large, we get

$$\lambda_2 \sim -\frac{1}{t_2 - t_1} \log \frac{E_{t_2}^+(\xi) - E_{t_2}^-(\xi)}{E_{t_1}^+(\xi) - E_{t_1}^-(\xi)}. \quad (19)$$

From the discussion of section III it should be clear how one applies (19) when the data of table 2 are available. One must see to it that ξ is so chosen that $\psi_2(\xi) \neq 0$, otherwise a higher eigenvalue may have been calculated. From the data of table 2 we obtain

$$\lambda_2 \sim 1.1,$$

whereas the exact value is $3/2 \sqrt{2} = 2.12$. The poor agreement could have been expected in view of low accuracy in the calculation of λ_1 .

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