Experiments on the Lattice Problem of Gauss

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1. Introduction. One of the classical unsolved problems in analytic number theory is concerned with counting the number of lattice points that lie in a circle. If A(r) is the number of lattice points in $\mathfrak{D}(r) \equiv \{(x, y) \mid x^2 + y^2 \leq r^2\}$ then the problem is to find the least value of θ such that

(1)
$$E(r) \equiv A(r) - \pi r^2 = O(r^{\theta}).$$

It has been shown by Loo-Keng Hua [1] that (1) holds for $\theta = \frac{13}{20}$ and by G. H. Hardy [2] that it does not hold for $\theta = \frac{1}{2}$. A conjecture, frequently attributed to Hardy, asserts that (1) is valid for all $\theta > \frac{1}{2}$.

The availability of high-speed digital computers suggests actually evaluating the deviation E(r) for "large" values of r in the hope of determining some further evidence of its behavior. At least three independent efforts in this direction have recently been made (as far as we know in the order: [3], [4], and the present paper). It is apparent from our results that the first effort [3] employed insufficiently large radii (r < 2000) and that the second effort [4] is incorrect for $r \ge 3000$. The present calculations, which extend to r = 259,750, suggest that (1) should be valid for some $\theta < \frac{13}{20}$. However, it also seems clear that the computations which would be required to approximate any such lower estimate are impractical on an IBM 7090 or even on any other currently existing computers.

A formula for computing A(r) is presented in Section 2. An efficient algorithm for evaluating this formula on a 7090 or similar machine and the corresponding program are described in Section 3. The numerical results are discussed in Section 4.

2. Formulation. For any positive real number Z, let [Z] denote the integer part of Z. For any radius r, we define the integers

(2)
$$K(r) \equiv [r/\sqrt{2}], \quad L(r) \equiv [r].$$

For all integers i in $K(r) + 1 \leq i \leq L(r)$ we define

(3)
$$y_i(r) \equiv \sqrt{r^2 - i^2}, \quad Y_i(r) = [y_i(r)]$$

If Q(r) is the number of lattice points in $\{(x, y) | x > 0, y > 0, x^2 + y^2 \le r^2\}$ then (see Figure 1)

(4)
$$Q(r) = K^{2}(r) + 2\sum_{i=K(r)+1}^{L(r)} Y_{i}(r).$$

The number of lattice points, A(r), in $\mathfrak{D}(r)$ can now be written as

(5)
$$A(r) = 4Q(r) + 4L(r) + 1.$$

The computing problem lies in the evaluation of $\sum Y_i$. It is relatively time

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FIG. 1. Diagram to explain the counting algorithm.

consuming to determine square roots on most existing computers and the accuracy required here is to within the integral part of y_i . There is in fact no serious problem for "small" values of r (say, $r < 2^{13} \doteq 8.2 \times 10^3$) either with regard to time or accuracy. However, if, as we desire, r^2 is of the order of magnitude of the machine fixed point word capacity ($2^{36} - 1$ on an IBM 7090) then efficiency and extreme accuracy are crucial. We shall describe a counting procedure to evaluate $\sum Y_i$ which employs no square root computations and is more efficient on a 7090 than any other procedure known to us. This procedure may not be the most efficient on a machine with a very fast fixed point square root instruction.

3. Counting Algorithm and Machine Program. Let 3(r) denote the set

 $\mathfrak{I}(r) \equiv \{(x, y) \mid y > 0; K + 1 \leq x \leq L; (x, y) \in \mathfrak{D}(r)\}.$

Then $\sum Y_i$ is just the number of lattice points contained in $\mathfrak{I}(r)$. If the lattice

point $(i, j) \in \mathfrak{I}(r)$ and the point $(i, j + 1) \notin \mathfrak{I}(r)$ then $Y_i(r) = j$. Furthermore, for such a lattice point (i, j), if i > K + 1 then, as a simple geometric or algebraic argument shows, $(i - 1, j + 1) \in \mathfrak{I}(r)$. Thus, roughly speaking, we can count the number of lattice points in $\mathfrak{I}(r)$ by tracing out a piecewise rectangular boundary which is just interior to the circular boundary of $\mathfrak{I}(r)$. This is done by starting at the point (i, j) = (L, 0) and with fixed *i* increasing *j* until $R_{i,j}^2 \equiv i^2 + j^2 > r^2$. When the first such *j* is obtained and $Y_i(r) = (j - 1)$ is accumulated in $\sum Y_i$ then reduce *i* by unity. Continue this procedure until i = K + 1. A great saving in computing time is effected by noting that

$$R_{i,j+1}^2 = R_{i,j}^2 + 2j + 1, \qquad R_{i-1,j}^2 = R_{i,j}^2 - 2i + 1.$$

Thus, on a binary machine, given $R_{L,0}^2$, no multiplications are required to evaluate recursively the $R_{i,j}^2$.

The algorithm for computing A(r) based on the above observations is described on the flow diagram, Figure 2. This algorithm was coded in FAP for the 7090. Using fixed-point machine operations the closed loop $1.0 \rightarrow 1.1 \rightarrow 1.2 \rightarrow 1.0$ takes 19 machine cycles while the partial loop $2.0 \rightarrow 2.1 \rightarrow 2.2 \rightarrow 1.2 \rightarrow 1.0$ requires 33 cycles. The first loop must be used for each j in $0 < j \leq K(r)$ or essentially $[r/\sqrt{2}] \doteq 0.7r$ times. The partial loop is used for each i in $K + 1 \leq i \leq L$ or essentially $[r] - [r/\sqrt{2}] \doteq 0.3r$ times. Since a 7090 machine cycle is about 2.18 microseconds, this code requires approximately $51r \times 10^{-6}$ seconds in order to compute A(r).

Using the 7090 fixed-point arithmetic operations a code based on the flow diagram of Figure 2 can compute A(r) for all $r < \sqrt{2} \times 2^{17} \doteq 1.8 \times 10^5$. By employing the sign bit to record arithmetic data the range of r is easily extended to $r < 2^{18} \doteq 2.6 \times 10^5$. In order to do this the ordinary arithmetic machine operations must be modified. The closed loop then takes 22 cycles and the partial loop only 32 cycles. The total time to compute A(r) then becomes $55r \times 10^{-6}$ sec. The time estimates given here were found to be extremely accurate.

For values of r such that $r^2 \doteq 2^{35}$ the arithmetic in boxes 0.1 and 3.0 of the flow diagram required special higher precision techniques which do not essentially alter the above time estimates. In fact, by using certain tricks only (Q + L) is required in the 7090 in order to calculate E and a special 1401 output routine can be used to transform (Q + L) in octal to A(r) in decimal.

It is a simple matter to employ the above procedures in order to count the number of lattice points in a sphere, say of radius ρ . We need only compute $A(r_k)$ where $r_k = \sqrt{\rho^2 - k^2}$ for $k = 0, 1, \dots, [\rho]$. Using the previous estimate this requires at least $55\left(\frac{\pi}{4}\right)\rho^2 \times 10^{-6}$ sec. for the total count.

4. Numerical Results. It is an elementary fact that A(r) is a piecewise constant function with discontinuities only at values of r for which r^2 can be written as the sum of the squares of two integers. Thus, for any integer m there are only a finite number of distinct values of A(r) for all $r \leq m$. However, it is quite impractical, for large m, to compute all of these values (e.g., for $m = 10^5$ we would require the order of 10^{10} computations). Hence, we content ourselves with some uniform samplings in r, bearing in mind the defects in any such experimental approach.



FIG. 2. Flow diagram for lattice point counting algorithm.

r	$A\left(r ight)$	E(r)	$\frac{\ln \mid E(r) \mid}{\ln r}$	$E(r)/r^{1/2}$
250000	196349539105	174436 04	.600532	34887201
250250	196742432789	- 349160 04	656313	-69797101
250500	197135722817	-15939204	593180	-31846601
250750	197529403589	- 16513204	595978	-32977001
251000	197923477597	-11718104	568341	-23389401
251000	198317943985	- 101137 04	556454	-20177101
251500	198712801597	-232602.04	623385	-46381501
251750	199108054785	-76375403	533784	-15221901
252000	199503696777	-30965604	646291	-61685001
252250	199899736189	-708459 03	527657	141058 01
252500	200296165009	-16114304	593679	- 320687 01
252750	200692987501	-154149.04	590065	-30661601
253000	201090202865	-12986204	576238	-25818101
253250	201487810273	-17108404	598349	-33996701
253500	201885812629	125849 03	388575	249955 00
253750	202284203409	-23125304	622471	-45907601
254000	202682990469	-11699904	567674	-23214901
254250	202002000100	-13465404	578921	-26704801
254500	203481740881	- 690174 03	525179	-13680901
254750	203481703117	-24688804	627530	-48015101
255000	200001100111	-18266704	603280	- 361735 01
255000	204202000415	-15235404	588658	-30156001
255500	201002010103	- 867505 03	543380	-171623 01
255750	205085352351	-110454 04	560028	- 236207 01
256000	205887414661	-14846604	586443	-29343101
256250	205007414001	-57786103	510620	-114154 01
256500	206602447577	-16861404	596569	- 332028 01
256750	2000002441011	- 897506 03	545897	-17712601
257000	207099050519	-24079504	625081	-47498601
201000	201433030103	.210150 01	.020001	.111000 01
250000.000000	196349539105	17443604	.600532	348872 01
.015625	196349565329	640554 02	.334675	12811000
.031250	196349589697	239750 03	.440864	479500 00
.046875	196349614641	.160553 03	.408603	.321106 00
.062500	196349639409	.384855 03	.478941	.769710 00
.078125	196349664377	.809155 03	.538729	.161831 01
.093750	196349688785	.673454 03	.523960	.134690 01
.109375	196349713721	.106575 04	.560891	.213150 01
.125000	196349737825	.626047 03	.518087	$.125209 \ 01$
.140625	196349761401	341657 03	.469362	68331500
.156250	196349787081	.794635 03	.537273	.158926 01
.171875	196349810921	$.909264 \ 02$.362858	.181852 00
.187500	196349835377	$.321620 \ 01$.093988	.643239 - 02
.203125	196349860537	.619504 03	.517242	.123900 01
.218750	196349885521	.105979 04	.560439	.211958 01
.234375	196349910209	.120407 04	.570709	.240815 01
.250000	196349934809	.126035 04	.574384	.252071 01
.265625	196349959225	.113264 04	.565788	.226528 01
.281250	196349983153	.516922 03	.502677	.103384 01
.296875	196350007041	138798 03	.396889	277596 00
.312500	196350031185	538520 03	.505971	107704 01

TABLE 1

r	A(r)	E(r)	$\frac{\ln \mid E(r) \mid}{\ln r}$	$E(r)/r^{1/2}$	
$\begin{array}{r} 250000.328125\\ .343750\\ .359375\\ .375000\\ .390625\\ .406250\\ .421875\\ .437500\\ .423125\\ .468750\\ .484375\\ .500000\end{array}$	$\begin{array}{c} 196350055801\\ 196350080809\\ 196350105305\\ 196350129513\\ 196350129513\\ 196350153921\\ 196350178761\\ 196350202577\\ 196350227629\\ 196350227629\\ 196350227597\\ 196350302053\\ 196350326845\end{array}$	$\begin{array}{c}466245 & 03 \\197063 & 01 \\496977 & 02 \\385426 & 03 \\521156 & 03 \\224888 & 03 \\952621 & 03 \\444356 & 03 \\ .371907 & 03 \\ .436169 & 03 \\ .348430 & 03 \\ .596689 & 03 \end{array}$	$\begin{array}{c} .494376\\ .054578\\ .314256\\ .479060\\ .503334\\ .435715\\ .551862\\ .490507\\ .476188\\ .489011\\ .470941\\ .514223\end{array}$	$\begin{array}{c}932489 \ 00 \\394127 - 02 \\993954 - 01 \\770852 \ 00 \\104231 \ 01 \\449776 \ 00 \\190524 \ 01 \\888711 \ 00 \\ .743813 \ 00 \\ .872338 \ 00 \\ .696859 \ 00 \\ .119337 \ 01 \end{array}$	
				1	

TABLE 1—Continued

TABLE 2

r	A(r)	E(r)	$\ln \mid E(r) \mid / \ \ln r$	$E(r)/r^{1/2}$
1000	3141549	436535 02	. 546673	138044 01
2000	12566345	256143 02	.426680	57275400
3000	28274197	136882 03	.614401	249911 01
4000	50265329	153457 03	.606871	242637 01
5000	78539677	139339 03	.579641	197056 01
6000	113097185	150529 03	.576372	194332 01
7000	153937805	235025 03	.616659	280909 01
8000	201061681	248829 03	.613847	278200 01
9000	254468477	527940 03	.688522	556498 01
10000	314159053	212358 03	.581767	212358 01
20000	1256636857	204435 03	.537210	144558 01
30000	2827432965	423230 03	.586666	244352 01
40000	5026547529	716743 03	.620453	35837101
50000	7853981045	588974 03	.589511	263397 01
60000	11309732881	671923 03	.591718	274311 01
70000	15393802989	101358 04	.620392	383100 01
80000	20106192121	861974 03	.598702	304754 01
90000	25446899381	111307 04	.614932	371025 01
100000	31415925457	10788904	.606596	341177 01
125000	49087384401	811340 03	. 570777	229481 01
150000	70685833345	136077 04	.605434	351349 01
175000	96211274253	763187 03	.549801	182436 01
200000	125663704421	17225904	.610481	385183 01
225000	159043126541	15469804	.595922	326132 01
250000	196349539105	17443604	.600532	348872 01



FIG. 3. Distribution of some computed values of $\ln |E(r)| / \ln r$.

Computations were made for each value of r in the following sets:

a) $r = 1(1)10,000$	g) $r = 200,000(1)200,099$
b) $r = 10,000(250)100,000$	h) $r = 250,000(1)250,099$
c) $r = 100,000(10,000)150,000$	i) $r = 100,000(\frac{1}{64})100,002$
d) $r = 150,000(250)259,750$	j) $r = 150,000(\frac{1}{64})150,002$
e) $r = 100,000(1)100,099$	k) $r = 200,000(\frac{1}{64})200,002$
f) $r = 150,000(1)150,099$	l) $r = 250,000(\frac{1}{64})250,002$

The quantities computed were: E(r), $E(r)/r^{1/2}$, $\ln |E(r)|/\ln r$, $\ln |E(r)/r^{1/2}|/\ln r$, and $E(r)/(r \ln r)^{1/2}$. The values of A(r) and E(r) were compared with all the values reported in [4]. Exact agreement for A(r) and agreement to at least five digits for E(r) was observed for r = 1(1)1,000 and r = 2,000. However, the remaining 27 values of A(r) for r in 3,000 $\leq r \leq 200,000$ reported in [4] did not agree with our values. Independent check calculations were made for r = 3000, = 4000, = 5000 by using equations (2)-(5). The square roots were evaluated by means of a Newton-Raphson subroutine and exact agreement for A(r) with those computed by the method of Section 3 was obtained. Thus, we conclude that the results in [4] are incorrect for $r \geq 3000$. We also believe that our calculations are correct for all reported values of r. Since our method depends upon r only through the quantities r^2 , K(r), and L(r) and then only integer arithmetic is performed on numbers which fit into a machine word, it seems quite likely that our claim is justified.

Table 1 lists a small sample of the numerical results from sets d) and l) and Table 2 lists sample results from sets a)-d). The numbers in the columns headed E(r) and $E(r)/r^{1/2}$ are in floating decimal notation with signed exponents and those in the A(r) column are integers. Positive values of E(r) were observed to be extremely rare for integer values of r. For example, in the approximately 890 cases contained in sets c)-h) only one such value was found, namely, r = 253,500. However, in the sets i)-l) the sign distribution of E(r) was about uniform or perhaps even slightly biased in favor of positive values.

In Figure 3 values of $\ln |E(r)|/\ln r$ vs. r are plotted on a semi-log scale. The dots have the abscissae: $r = 3000(200)6000(500)2 \times 10^4(10^3)3 \times 10^4(2 \times 10^3)6 \times 10^4(5 \times 10^3)2 \times 10^5(10^4)2.6 \times 10^5$. The horizontal lines in Figure 3 of ordinate 0.5 and 0.65 represent respectively Hardy's lower bound and Hua's upper bound on the order θ in equation (1). The points marked with an X in Figure 3 were plotted to indicate that not all values computed for $r > 10^5$ were below Hua's bound. Many such values of $\ln |E(r)|/\ln r > 0.65$ were obtained in the sets i)-l) at non-integral values of r. The largest such value observed in $10^5 \leq r \leq 259,750$ was 0.672 at r = 103,000.

The results summarized in Figure 3 clearly suggest that (1) is valid for $\theta = 0.70$ or even perhaps for $\theta = 0.68$. But since it is known to be valid for all $\theta \ge 0.65$ no useful quantitative estimates are obtained. However, an extrapolation of these data does suggest that a smaller order should suffice and that computations for larger values of r could indicate this. For example, to obtain a significant improvement, say $\theta \le 0.60$, a crude extrapolation implies a radius of about 10⁸. Unfortunately, calculations for such radii, employing a partial-double-precision version of our present method on a 7090, would require at least two hours per case. Hence, they are impractical for the number of cases required to show a reasonable trend in the data. Furthermore, serious problems arise in attempting to insure the accuracy of such computations.

It was also observed that for all of our calculations $|E(r)|/r^{1/2} < 7$. Since by Hardy's result this ratio is unbounded we must conclude that either our sampling is too crudely spaced or more likely that our range in r is relatively small.

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