Will my numbers add up correctly if I round them?

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I recently wrote a solution to a student problem. The answers were the probabilities for four possible outcomes. As a check on the calculations, I wanted to say 'As expected, these probabilities add up to 1.' However, they didn't! Because of rounding, the probabilities (which I was quoting to four decimal places) only added up to 0.9999. To rescue the situation I tried rounding to 3DP or 5DP instead, but these didn't add up correctly either. (See Table 1.)

Exact values (not rounded)	Rounded to … 2DP	3DP	4DP	5DP
0.2979493…	0.30	0.298	0.2979	0.29795
0.3724367…	0.37	0.372	0.3724	0.37244
0.2333670…	0.23	0.233	0.2334	0.23337
0.0962470…	0.10	0.096	0.0962	0.09625
Total = 1	1.00 ✓	0.999 ✘	0.9999 ✘	1.00001 ✘

TABLE 1: Rounding to different numbers of decimal places

A similar issue often arises in opinion polls where the rounded percentages of people answering 'Yes', 'No' and 'Don't know', e.g. 64%, 25% and 10%, don't add up to 100%.

So I wondered how likely it is that a set of n random numbers will add up correctly when the individual numbers and the total are rounded to d decimal places. When does 'round then sum' give the same answer as 'sum then round'?

I will show here that, based on some simple assumptions, the probability that the rounding works correctly is equal to $\frac{2}{\pi}\int_0^\infty \left(\frac{\sin x}{x}\right)^{n+1} dx$. It is perhaps surprising that such an exotic integral should arise in a real-world problem and that these probabilities take rational values, as shown in Table 2. A detailed description of this type of integral was given in an earlier *Gazette* article [1].

$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$
1	$\frac{3}{4}$	$\frac{2}{3}$	$\frac{115}{192}$	$\frac{11}{20}$	$\frac{5887}{11520}$	$\frac{151}{315}$	$\frac{259723}{573440}$
1.0000	0.7500	0.6667	0.5990	0.5500	0.5110	0.4794	0.4529

TABLE 2: Probabilities for small values of n

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I will assume in my model that the fractional parts of the numbers involved can be considered to come from a continuous uniform distribution. Provided that a few significant figures still remain after rounding and the numbers don't have a special form, this will be a reasonable assumption in many situations. Even if the numbers follow a different distribution such as Benford's Law [2], which real-life lists of numbers often conform to, the distribution of the third and higher significant digits will be practically indistinguishable from a uniform distribution. In my example the probabilities involved sums of exponential functions. Note, however, that this assumption may not be valid in some cases, e.g. if the probabilities come from a binomial distribution in which the probability p takes a rational value.

Initial observations

To start with, note that if we multiply the four exact (unrounded) values in Table 1 by 10 000, then round each of the resulting values to the nearest integer and calculate the total (9999), this is effectively the same calculation as rounding to 4DP. The digits in the 'Nearest integer' column in Table 3 match the digits in the 4DP column in Table 1.

Exact value	× 10 000	Nearest integer	Fractional part
0.2979493…	2979.493…	2979	0.493…
0.3724367…	3724.367…	3724	0.367…
0.2333670…	2333.670…	2334	0.670…
0.0962470…	962.470…	962	0.470…
Total = 1	10000	9999	2.000…

TABLE 3: The equivalent problem involving integers

This tells us several things:

(1) If we can assume that the fractional parts of the original exact values are uniformly distributed (with the digits going on for ever), this will also be true of the new fractional parts after we multiply by *any* power of 10. So the probability that the rounding will work correctly when the numbers are added is independent of the number of decimal places d we round to.

(2) We can therefore just consider whether rounding numbers such as those in the second column of Table 3 (2979.493… etc.) to the nearest integer (2979 etc.) will give the correct total. (Here $9999 \neq 10\,000$, so they don't.) Furthermore, the particular values of the integer parts appearing in this calculation (2979 etc.) do not affect the direction of the rounding, i.e. whether the fractional parts round up or down. So, without loss of generality, we can assume that the integer parts are all zero, i.e. we can just consider numbers such as those in the final column of Table 3 (0.493… etc.), which lie in the range $[0, 1)$.

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(3) If the fractional parts come from a continuous uniform distribution there should be no link between the digits featuring at different positions. So the rounding errors arising from rounding to different numbers of decimal places will be statistically independent. This means that we can work out the probability that the rounding will not work correctly based on several levels of precision, e.g. for 3DP *and* 4DP *and* 5DP, by just multiplying the relevant probabilities together.

(4) If we write the exact values in a different base (e.g. binary), the numbers we obtain after rounding will in general be different. However, the fractional parts will still be uniformly distributed. So the probability that the totals round correctly is still the same, irrespective of the number base used.

Mathematical specification

I have adopted the following mathematical model. Let $u_1, u_2, \ldots, u_n$ be independent random numbers distributed uniformly on $[0, 1)$ and let $N(x) = \left[x + \frac{1}{2}\right]$ denote the function that rounds to the nearest integer. The error ε in the final digit due to rounding will then be

$$\varepsilon = \sum_{i=1}^{n} N(u_i) - N\left(\sum_{i=1}^{n} u_i\right).$$

This is 'round then sum' minus 'sum then round'. For example, in the 4DP example above, we have

$$\sum_{i=1}^{4} N(u_i) = N(0.493) + N(0.367) + N(0.670) + N(0.470) = 0 + 0 + 1 + 0 = 1$$

and $$N\left(\sum_{i=1}^{4} u_i\right) = N(0.493 + 0.367 + 0.670 + 0.470) = N(2.000) = 2.$$

So in this case the error is $\varepsilon = 1 - 2 = -1$. If $\varepsilon = 0$, the rounding works correctly and I will write the probability of this outcome as $p(n)$.

This model ignores the fact that the theoretical total is often an exact prescribed number, e.g. 1 or 100%, as in the examples above. In this case the value of one of the 'random' numbers is forced. For example, the number 0.0962470… in Table 1 can be deduced exactly from the other three values. (In statistical terminology we 'lose one degree of freedom'.) To deal with this situation, in the formulae derived below we just need to replace n with $n - 1$ (the number of *independent* values).

Small values of n

If $n = 1$, the total is just equal to the single original value. So, trivially, the total will always be correct after rounding. So $p(1) = 1$.

If $n = 2$, we can use the diagram in Figure 1 to find the probability that the total will be correct after rounding. The axes show the fractional parts

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u_1 and u_2, and the numbers shown in the triangles are the corresponding rounding errors ε. For example, the point indicated is $(0.2,\ 0.4)$ and the error for this point is $\varepsilon = [N(0.2) + N(0.4)] - N(0.6) = 0 - 1 = -1$.

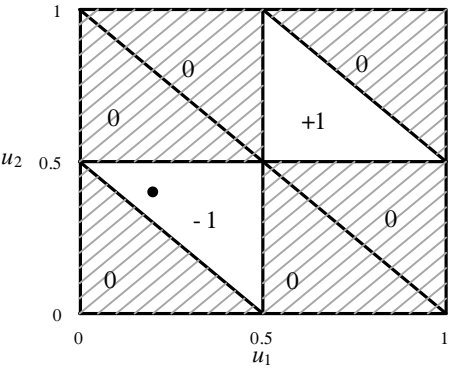


FIGURE 1: Rounding errors with two numbers

We can see that the probability that the rounding will work correctly is $\frac{3}{4}$ (corresponding to the proportion of the square that is shaded), and that there is a probability of $\frac{1}{8}$ that we will get a rounding error of 1 unit in either direction. So $p(2) = \frac{3}{4}$.

Sums of uniform distributions

To extend these results to higher values of n, which are not easy to visualise geometrically, I will need to use some results relating to the sums of uniform distributions.

If $U_1, U_2, \ldots, U_n$ are independent $U(0,\ 1)$ random variables, then the probability density function of $Y = \sum_{i=1}^{n} U_i$, is

$$f_n(y) = \frac{1}{(n-1)!} \sum_{j=0}^{[y]} (-1)^j \binom{n}{j} (y-j)^{n-1}, \qquad 0 \leqslant y < n. \qquad (1)$$

This can be established by starting from $f_1(y) = 1,\ 0 \leqslant y < 1$ and repeatedly applying the convolution equation $f_n(y) = \int_{y-1}^{y} f_{n-1}(t)\,dt$, paying careful attention to the limits of the integrals involved. Equation (1) can then be confirmed by induction.

Since the rounding of each number depends on whether it is greater than or less than $\frac{1}{2}$, we will actually need to use the PDF of the related quantity $X = \sum_{i=1}^{n} V_i$, where $V_1, V_2, \ldots, V_n$ are independent $U\left(0,\ \frac{1}{2}\right)$ random variables, i.e. they are uniform over the range $[0,\ \frac{1}{2})$. Since values of V_i can be obtained by simply halving the values of U_i, thus transforming the $U(0,\ 1)$ distribution into a $U\left(0,\ \frac{1}{2}\right)$ distribution, we can find the PDF of X by applying the transformation $X = \frac{1}{2}Y$ to (1). This tells us that the PDF of

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X is

$$g_n(x) = 2f_n(2x) = \frac{2}{(n-1)!}\sum_{j=0}^{[2x]}(-1)^j\binom{n}{j}(2x-j)^{n-1}, \qquad 0 \leqslant x < \tfrac{1}{2}n. \quad (2)$$

This gives a piecewise continuous function with 'joins' at the half-integers $0, \frac{1}{2}, 1, \ldots, \frac{1}{2}n - \frac{1}{2}$. For example, for $n = 4$,

$$g_4(x) = \frac{1}{3}\sum_{j=0}^{[2x]}(-1)^j\binom{4}{j}(2x-j)^3 = \begin{cases} \frac{8}{3}x^3 & \text{if } 0 \leqslant x < \frac{1}{2} \\ \frac{4}{3} - 8x + 16x^2 - 8x^3 & \text{if } \frac{1}{2} \leqslant x < 1 \\ -\frac{44}{3} + 40x - 32x^2 + 8x^3 & \text{if } 1 \leqslant x < \frac{3}{2} \\ \frac{64}{3} - 32x + 16x^2 - \frac{8}{3}x^3 & \text{if } \frac{3}{2} \leqslant x < 2 \end{cases}$$

Figure 2 shows graphs of this function for a selection of values of n.

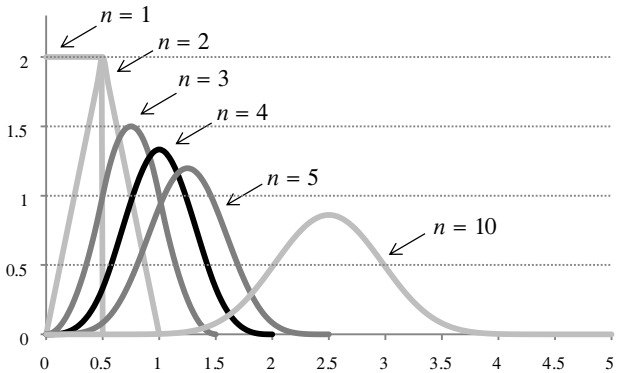


FIGURE 2: PDFs of the sum of n independent $U\left(0, \frac{1}{2}\right)$ random variables

Higher values of n

I will use the case $n = 4$ to show how we can find the probabilities $p(n)$ for higher values of n.

There is a probability of $\left(\frac{1}{2}\right)^4 = \frac{1}{16}$ that the fractional parts of the four numbers u_1, u_2, u_3, u_4 will all lie in the range $[0, \frac{1}{2})$, corresponding to the shaded areas in Figure 3. Because these values are all in the range $[0, \frac{1}{2})$, we

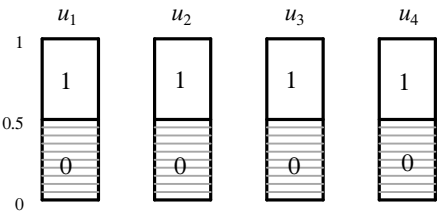


FIGURE 3: When all four fractional parts lie in the range $[0, \frac{1}{2})$

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have $N(u_1) + N(u_2) + N(u_3) + N(u_4) = 0$. So, in this case, the rounding will work correctly if $N(u_1 + u_2 + u_3 + u_4) = 0$, i.e. if $u_1 + u_2 + u_3 + u_4$ lies in the range $[0, \frac{1}{2})$. The probability of this outcome is $\frac{1}{16}\int_0^{1/2} g_4(x)\,dx$.

Another possibility is that the fractional parts fall in the ranges shown in Figure 4, with two values (u_2 and u_3, say) above $\frac{1}{2}$ and the other two below. In this case we have $N(u_1) + N(u_2) + N(u_3) + N(u_4) = 0 + 1 + 1 + 0 = 2$. So the rounding will work correctly if $N(u_1 + u_2 + u_3 + u_4) = 2$, i.e. if $u_1 + u_2 + u_3 + u_4$ lies in the range $[1\frac{1}{2}, 2\frac{1}{2})$.

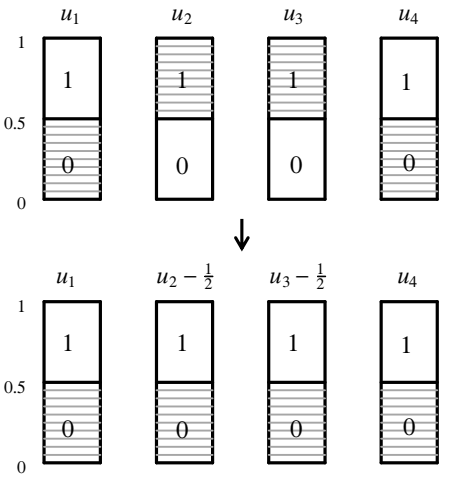


FIGURE 4: Dealing with other patterns

We can evaluate this probability using the same distribution as for the first case by noting that, if u_2 and u_3 are uniformly distributed on $[\frac{1}{2}, 1)$, then $u_2^* = u_2 - \frac{1}{2}$ and $u_3^* = u_3 - \frac{1}{2}$ are uniformly distributed on $[0, \frac{1}{2})$. We then have $N(u_1) + N(u_2^*) + N(u_3^*) + N(u_4) = 0$ and we need $u_1 + u_2^* + u_3^* + u_4$ to be in the range $[\frac{1}{2}, 1\frac{1}{2})$. This is then the same situation as in Figure 3, but with a different range for the total.

The pattern in Figure 4 can occur in $\binom{4}{2} = 6$ ways, because the two higher values could occur in any of the four positions. So the probability for this case is $\frac{6}{16}\int_{1/2}^{3/2} g_4(x)\,dx$.

If we fill in the other combinations in the same way, we find that the probability that the rounding will work correctly when $n = 4$ is

$$p(4) = \frac{1}{16}\int_0^{1/2} g_4(x)dx + \frac{4}{16}\int_0^{1} g_4(x)dx + \frac{6}{16}\int_{1/2}^{3/2} g_4(x)dx + \frac{4}{16}\int_1^{2} g_4(x)dx + \frac{1}{16}\int_{3/2}^{2} g_4(x)dx. \tag{3}$$

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The three middle integrals each cover a range of width 1 and include a 'join' in the function. If we split these up into two parts, e.g. $\int_0^1 = \int_0^{1/2} + \int_{1/2}^1$, we can write this result in the equivalent form

$$p(4) = \frac{5}{16}\int_0^{1/2} g_4(x)dx + \frac{10}{16}\int_{1/2}^{1} g_4(x)dx + \frac{10}{16}\int_1^{3/2} g_4(x)dx + \frac{5}{16}\int_{3/2}^{2} g_4(x)dx. \quad (4)$$

The adjacent coefficients of the form $\binom{4}{k-1}$ and $\binom{4}{k}$ in (3) combine to produce the coefficients of the form $\binom{5}{k}$ in (4). The general formula for this result is

$$p(n) = \frac{1}{2^n}\sum_{k=1}^{n}\binom{n+1}{k}\int_{(k-1)/2}^{k/2} g_n(x)\,dx. \quad (5)$$

Substituting for $g_n(x)$ from (2), we can write this as

$$p(n) = \frac{1}{2^n}\sum_{k=1}^{n}\binom{n+1}{k}\int_{(k-1)/2}^{k/2}\left(\frac{2}{(n-1)!}\sum_{j=0}^{k-1}(-1)^j\binom{n}{j}(2x-j)^{n-1}\right)dx. \quad (6)$$

Note that, since x takes values in the range $\frac{1}{2}(k-1) \leqslant x \leqslant \frac{1}{2}k$ in this integral, the upper limit for the summation over j becomes $\lfloor 2x \rfloor = k-1$.

Since

$$\int_{(k-1)/2}^{k/2}(2x-j)^{n-1}dx = \frac{1}{2n}\left\{(k-j)^n - (k-1-j)^n\right\},$$

this becomes

$$p(n) = \frac{1}{2^n n!}\sum_{k=1}^{k-1}\binom{n+1}{k}\sum_{j=0}^{k-1}(-1)^j\binom{n}{j}\left\{(k-j)^n - (k-1-j)^n\right\}.$$

The inner summation over j has the form of a telescoping sum, which we can simplify by changing the dummy variable in the second component to $j^* = j+1$, renaming j^* as j, combining the two components and simplifying.

$$\begin{aligned}
&\sum_{j=0}^{k-1}(-1)^j\binom{n}{j}(k-j)^n - \sum_{j=0}^{k-1}(-1)^j\binom{n}{j}(k-1-j)^n \\
&= \sum_{j=0}^{k-1}(-1)^j\binom{n}{j}(k-j)^n - \sum_{j^*=1}^{k}(-1)^{j^*-1}\binom{n}{j^*-1}(k-j^*)^n \\
&= \sum_{j=0}^{k-1}(-1)^j\binom{n}{j}(k-j)^n + \sum_{j=1}^{k}(-1)^j\binom{n}{j-1}(k-j)^n \\
&= \binom{n}{0}k^n + \sum_{j=1}^{k-1}(-1)^j\left\{\binom{n}{j} + \binom{n}{j-1}\right\}(k-j)^n + 0
\end{aligned}$$

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$$= \binom{n+1}{0} k^n + \sum_{j=1}^{k-1} (-1)^j \binom{n+1}{j} (k-j)^n$$

$$= \sum_{j=0}^{k-1} (-1)^j \binom{n+1}{j} (k-j)^n.$$

So (6) simplifies to

$$p(n) = \frac{1}{2^n n!} \sum_{k=1}^{n} \binom{n+1}{k} \sum_{j=0}^{k-1} (-1)^j \binom{n+1}{j} (k-j)^n. \tag{7}$$

By writing $r = k - j$ to group the terms with equal powers together, this can also be expressed in the alternative, but equivalent, form

$$p(n) = \frac{1}{2^n n!} \sum_{r=1}^{n} r^n \sum_{j=0}^{n-r} (-1)^j \binom{n+1}{j} \binom{n+1}{r+j}. \tag{8}$$

The numerical values in Table 2 above were calculated using this formula.

Simplifying the formula

Equation (8) involves a double sum of a long series of terms with alternating signs, resulting in fractions with rapidly increasing denominators. Evaluating these for larger values of n is not easy. However, we can simplify (8) considerably using some further tricks.

If we first add and subtract the next term in the inner sum (corresponding to $j = n - r + 1$), we have

$$p(n) = \frac{1}{2^n n!} \sum_{r=1}^{n} r^n \left\{ \sum_{j=0}^{n-r+1} (-1)^j \binom{n+1}{j} \binom{n+1}{r+j} - (-1)^{n-r+1} \binom{n+1}{n-r+1} \binom{n+1}{n+1} \right\}$$

$$= \frac{1}{2^n n!} \sum_{r=1}^{n} r^n \left\{ \sum_{j=0}^{n-r+1} (-1)^j \binom{n+1}{j} \binom{n+1}{r+j} - (-1)^{n-r+1} \binom{n+1}{r} \right\}. \tag{9}$$

We can then simplify the first component by noting that

$$\sum_{j=0}^{n-r+1} (-1)^j \binom{n+1}{j} \binom{n+1}{r+j}$$

is the coefficient of t^{n-r+1} when we multiply together the series expansions for $(1-t)^{n+1}$ and $(1+t)^{n+1}$. Since $(1-t)^{n+1}(1+t)^{n+1} = (1-t^2)^{n+1}$, this must equal the coefficient of t^{n-r+1} in $(1-t^2)^{n+1}$, so that

$$\sum_{j=0}^{n-r+1} (-1)^j \binom{n+1}{j} \binom{n+1}{r+j} = \begin{cases} (-1)^{(n-r+1)/2} \binom{n+1}{\frac{1}{2}(n-r+1)} & \text{if } n-r+1 \\ & \text{is even,} \\ 0 & \text{otherwise.} \end{cases}$$

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We can also simplify the second component of (9) by noting that r^n is an nth order polynomial and $\sum_{r=1}^{n+1} r^n(-1)^r\binom{n+1}{r}$ is an $(n+1)$th difference of this function. This must equal zero, in the same way that the third differences of a quadratic function are all equal to zero. So $\sum_{r=1}^{n+1} r^n(-1)^r\binom{n+1}{r} = 0$ and, separating out the term for $r = n+1$, we get

$$\sum_{r=1}^{n} r^n(-1)^r\binom{n+1}{r} = (-1)^n(n+1)^n$$

and hence

$$-\sum_{r=1}^{n} r^n(-1)^{n-r+1}\binom{n+1}{r} = (n+1)^n.$$

If we substitute these results into (9), we get

$$p(n) = \frac{1}{2^n n!}\left\{\sum_{\substack{r=1 \\ n-r+1 \text{ even}}}^{n} r^n(-1)^{(n-r+1)/2}\binom{n+1}{\frac{1}{2}(n-r+1)} + (n+1)^n\right\}.$$

If we then write $n - r + 1 = 2i$ in the sum to pick up the terms with the correct parity, this gives us the following simpler formula, which involves only a single summation

$$p(n) = \frac{1}{2^n n!}\left\{\sum_{i=1}^{[\frac{1}{2}n]}(n+1-2i)^n(-1)^i\binom{n+1}{i} + (n+1)^n\right\}$$

$$= \frac{1}{n!}\sum_{i=1}^{[\frac{1}{2}n]}\left(\tfrac{1}{2}(n+1)-i\right)^n(-1)^i\binom{n+1}{i}. \qquad (10)$$

I have used (10) in *Mathematica* to calculate accurate values for powers of 10 up to $n = 10^5$. These are shown to 10 decimal places in Table 4. (The approximate values are derived from the asymptotic result in (14) below.)

$p(n)$	$n = 10$	$n = 100$	$n = 1000$	$n = 10\,000$	$n = 100\,000$
Accurate	0.4109626428	0.1373074303	0.0436735567	0.0138188678	0.0043701653
Approx	0.4109626675	0.1373074303	0.0436735567	0.0138188678	0.0043701653

TABLE 4: Accurate and approximate values of $p(n)$ for powers of 10

I am grateful to the referee for drawing my attention to a paper from 1987 [3], which also derived (10), using a different method, and included an almost identical diagram to my Figure 1.

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The integral connection

The connection with the sine integral arises because we can also express $\int_0^\infty \left(\frac{\sin x}{x}\right)^n dx$ in terms of a similar summation formula.

In [1, p. 217] the author shows that

$$\int_0^\infty \frac{\sin^n x}{x^m}\,dx \;=\; \frac{1}{(m\,-\,1)!}\int_0^\infty \left(\frac{1}{x}\,\frac{d^{m-1}}{dx^{m-1}}\left(\sin^n x\right)\right)dx.$$

This leads to the following results (given in the Appendix on p. 222):

$$\int_0^\infty \frac{\sin^n x}{x^m}\,dx = \begin{cases} \dfrac{\pi}{(m-1)!}\left(\dfrac{1}{2}\right)^n \displaystyle\sum_{k=1}^{r}(-1)^{k+q}\binom{n}{r-k}(2k)^{m-1} & (n=2r,\ m=2q) \\[2ex] \dfrac{\pi}{(m-1)!}\left(\dfrac{1}{2}\right)^n \displaystyle\sum_{k=0}^{r}(-1)^{k+q}\binom{n}{r-k}(2k+1)^{m-1} & (n=2r+1,\ m=2q+1) \end{cases}$$

If we set $q = r$ and use the substitution $i = r - k$ (or $k = r - i$), these two forms become

$$\begin{aligned}\int_0^\infty \frac{\sin^{2r} x}{x^{2r}}\,dx &= \frac{\pi}{(2r-1)!}\left(\frac{1}{2}\right)^{2r}\sum_{i=0}^{r-1}(-1)^{2r-i}\binom{2r}{i}(2r-2i)^{2r-1} \\ &= \frac{\pi}{2}\frac{1}{(2r-1)!}\sum_{i=0}^{r-1}(-1)^{i}\binom{2r}{i}(r-i)^{2r-1}\end{aligned}$$

and

$$\begin{aligned}\int_0^\infty \frac{\sin^{2r+1} x}{x^{2r+1}}\,dx &= \frac{\pi}{(2r)!}\left(\frac{1}{2}\right)^{2r+1}\sum_{i=0}^{r}(-1)^{2r-i}\binom{2r+1}{i}(2r-2i+1)^{2r} \\ &= \frac{\pi}{2}\frac{1}{(2r)!}\sum_{i=0}^{r}(-1)^{i}\binom{2r+1}{i}(r+\tfrac{1}{2}-i)^{2r}.\end{aligned}$$

These can be combined in the form

$$\int_0^\infty \frac{\sin^n x}{x^n}\,dx \;=\; \frac{\pi}{2}\frac{1}{(n-1)!}\sum_{i=0}^{[(n-1)/2]}(-1)^{i}\binom{n}{i}(\tfrac{1}{2}n-i)^{n-1}.$$

Comparing this with (10), we see that

$$p(n) \;=\; \frac{2}{\pi}\int_0^\infty \left(\frac{\sin x}{x}\right)^{n+1} dx. \tag{11}$$

These integrals can be expressed in various alternative forms. For example, [4] shows that

$$\int_0^\infty \left(\frac{\sin x}{x}\right)^n dx = \begin{cases} n\displaystyle\int_0^\infty \frac{u^{n-2}}{(u^2+2^2)(u^2+4^2)\ldots(u^2+n^2)}\,du & (n\,\text{even}) \\[2ex] n\displaystyle\int_0^\infty \frac{u^{n-1}}{(u^2+1^2)(u^2+3^2)\ldots(u^2+n^2)}\,du & (n\,\text{odd}) \end{cases}$$

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Note that the power in the numerator is $n - 2$ in the first case, but $n - 1$ in the second case. However, we can write these integrals in a slightly more consistent form by applying the substitution $y = 1/u$.

$$\int_0^\infty \left(\frac{\sin x}{x}\right)^n dx = \begin{cases} n\int_0^\infty \dfrac{1}{(1+2^2y^2)(1+4^2y^2)\ldots(1+n^2y^2)}\,du & (n \text{ even}) \\ n\int_0^\infty \dfrac{1}{(1+1^2y^2)(1+3^2y^2)\ldots(1+n^2y^2)}\,du & (n \text{ odd}) \end{cases}$$

Distribution of the errors

By adjusting the ranges of the integrals in (3) we can modify the method above to find $p(n, \varepsilon)$, the probability distribution for the different sizes of error ε that can result from rounding. This gives a rather unwieldy generalisation of (6).

$$p(n,\varepsilon) = \frac{1}{2^{n-1}(n-1)!} \sum_{k=\max(0,1-2\varepsilon)}^{\min(n+1,n-2\varepsilon)} \binom{n+1}{k} \int_{\frac{1}{2}k+\varepsilon-\frac{1}{2}}^{\frac{1}{2}k+\varepsilon} \sum_{j=0}^{k+2\varepsilon-1} (-1)^j \binom{n}{j} (2x-j)^{n-1}\,dx.$$

This applies for values of $n = 1, 2, 3, \ldots$ and $\varepsilon = -\left[\frac{1}{2}n\right], \ldots, -2, -1, 0, 1, 2, \ldots \left[\frac{1}{2}n\right]$.

As before, we can simplify this using the same tricks described above to obtain the following simpler formula (which reduces to (10) when $\varepsilon = 0$):

$$p(n, \varepsilon) = \frac{1}{n!} \sum_{i=0}^{\left[\frac{1}{2}n-\varepsilon\right]} \left(\tfrac{1}{2}(n+1) - \varepsilon - i\right)^n (-1)^i \binom{n+1}{i}. \qquad (12)$$

The values for $n = 4$, calculated using this formula, are shown in Table 5 below. As we would expect, the probabilities for the errors form a symmetrical distribution about zero.

I suspected that (12) could also be expressed in the form of a sine integral by generalising (11) in some way, but I couldn't see how to achieve this. I am grateful once again to the referee for suggesting an alternative method of deriving these results based on more advanced statistical theory. He noted that $p(n)$ could be expressed in terms of a sum of $U(-1,1)$ random variables, each of which has characteristic function $\dfrac{\sin t}{t}$. This insight has enabled me to establish that $p(n, \varepsilon)$, the probability of obtaining a rounding error of ε, can be expressed in the form

$$p(n, \varepsilon) = \int_{2\varepsilon-1}^{2\varepsilon+1} \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\frac{\sin t}{t}\right)^n e^{-itz} dt \right\} dz.$$

This can be simplified (with t renamed as x) to give the general formula

$$p(n, \varepsilon) = \frac{2}{\pi} \int_{-\infty}^{\infty} \left(\frac{\sin x}{x}\right)^n \cos 2\varepsilon x\, dx. \qquad (13)$$

This generalisation 'works' because, when $|\varepsilon| > \frac{1}{2}(n+1)$, this integral evaluates to zero (even for non-integer values of ε), which I don't think is immediately obvious.

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Some experimental results

Checking the answers

To check these results, we can calculate the rounding errors in the totals when the four 'random' numbers $\pi = 3.14159\ldots$, $e = 2.71828\ldots$, $\sqrt{2} = 1.41421\ldots$ and $\phi = 1.61803\ldots$ are rounded to d decimal places for different values of d. Table 5 shows the distribution of errors for all values of d in the range 1,2,3, … ,115 200. (The upper limit for d was chosen so that the expected numbers were all multiples of 100 and the calculations would take less than 5 hours to run on my computer in *Mathematica*!)

Error in the final digit (ε)	−2	−1	0	1	2
Theoretical proportion, calculated using (12) with $n = 4$	$\frac{1}{384}$	$\frac{19}{96}$	$\frac{115}{192}$	$\frac{19}{96}$	$\frac{1}{384}$
Actual number of occurrences	312	22 863	68 915	22 807	303
Expected number of occurrences	300	22 800	69 000	22 800	300

TABLE 5: Checking the results

These results have a chi-square value of $\chi^2 = \sum \frac{(\text{Actual} - \text{Expected})^2}{\text{Expected}} = 0.79$, based on 4 degrees of freedom. The low value of 0.79 indicates that the actual numbers are entirely consistent with the expected numbers predicted by (12).

Asymptotic formulae

From Table 4 it appears that increasing n by a factor of 100 reduces the value of $p(n)$ by a factor of approximately 10, suggesting that asymptotically $p(n) \approx k/\sqrt{n}$. Looking at the numerical values of $p(n)\sqrt{n}$ further suggests that $k = \sqrt{6/\pi} = 1.38197659\ldots$.

This approximation can be refined further by looking for an asymptotic series of the form

$$p(n-1) = \frac{2}{\pi}\int_0^\infty \left(\frac{\sin x}{x}\right)^n dx \approx \sqrt{\frac{6}{\pi n}}\left(1 + \frac{a_1}{n} + \frac{a_2}{n^2} + \frac{a_3}{n^3} + \frac{a_4}{n^4}\right).$$

(I've used $n-1$ here, rather than n, so that the power in the sine integral is n.)

The values of a_1, a_2, a_3, a_4 can be found iteratively by calculating $p(n)$ very accurately for a few large values of n and using simultaneous equations to identify the successive coefficients, assuming that the denominators will be one of the 'usual suspects'. This leads to (14), which gives very accurate approximations (see Table 4).

$$p(n-1) = \sqrt{\frac{6}{\pi n}}\left(1 - \frac{3}{20n} - \frac{13}{1120n^2} + \frac{27}{3200n^3} + \frac{52\,791}{3\,942\,400n^4} + O\left(n^{-5}\right)\right). \quad (14)$$

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Generating functions

Another way to check the results and look for further connections is to find a generating function. After some experimenting, I have found that the values of $p(n, \varepsilon)$ can be captured as the coefficients of the following function:

$$G(x, t) = \sum_{n=0}^{\infty} \sum_{\varepsilon=-\left[\frac{1}{2}n\right]}^{\left[\frac{1}{2}n\right]} p(n, \varepsilon) x^{\varepsilon} t^n = \frac{y \cosh yt}{y - \sinh yt},$$

where $y = \frac{1}{2}\left(\sqrt{x} - \frac{1}{\sqrt{x}}\right) = \sinh\left(\frac{1}{2} \ln x\right)$.

For example, to obtain the terms up to t^4, we can use the *Mathematica* code

```
Series[y*Cosh[y*t]/(y-Sinh[y*t])/.y->(Sqrt[x]-1/Sqrt[x])/2,{t,0,4}]
```

This generates a series of the form

$$G(x, t) = 1 + t + \left(\tfrac{1}{8}x^{-1} + \tfrac{3}{4} + \tfrac{1}{8}x\right)t^2 + \left(\tfrac{1}{6}x^{-1} + \tfrac{2}{3} + \tfrac{1}{6}x\right)t^3 + \left(\tfrac{1}{384}x^{-2} + \tfrac{19}{96}x^{-1} + \tfrac{115}{192} + \tfrac{19}{96}x^{1} + \tfrac{1}{384}x^{2}\right)t^4 + \ldots \quad (15)$$

The t^4 term reproduces the numerical values of $p(4, \varepsilon)$ shown in Table 5.

Based on this generating function, we can also confirm that, for each value of n, the probabilities for $p(n, \varepsilon)$ sum to 1, since

$$\sum_{n=0}^{\infty} \sum_{\varepsilon=-\left[\frac{1}{2}n\right]}^{\left[\frac{1}{2}n\right]} p(n,\varepsilon)t^n = \lim_{x\to 1} G(x,t) = \lim_{y\to 0} \frac{\cosh yt}{1 - \dfrac{\sinh yt}{y}} = \frac{1}{1-t} = \sum_{n=0}^{\infty} 1t^n.$$

So they define a valid probability distribution.

Also, evaluating $\lim_{x \to 1} \dfrac{\partial^2}{\partial^2 x} G(x, t)$ using *Mathematica* shows that $\sum \varepsilon^2 p(n, \varepsilon)$, the variance of the errors, is equal to $\frac{1}{12}(n + 1)$ when $n \geqslant 2$. So when $n \leqslant 10$, the standard deviation will be less than 1 and the rounding errors will typically be quite small.

The coefficient of x^0 in (15) gives a generating function for the values of $p(n)$,

$$G(t) = \textstyle\sum_{n=0}^{\infty} p(n)t^n = 1 + t + \frac{3}{4}t^2 + \frac{2}{3}t^3 + \frac{115}{192}t^4 + \frac{11}{20}t^5 + \frac{5887}{11520}t^6 + \frac{151}{315}t^7 + \ldots \quad (16)$$

The simplest formula I have been able to find for this series is

$$G(t) = \frac{1}{n} \sum_{k=0}^{n-1} g\left(\sin \frac{k\pi}{n}, t\right) + O\left(t^{2n}\right) \text{ for } n = 1,2,3, \ldots \quad (17)$$

where $g(\alpha, t) = \begin{cases} \dfrac{\alpha \cos \alpha t}{\alpha - \sin \alpha t} & \text{if } \alpha \neq 0, \\ \dfrac{1}{1 - t} & \text{if } \alpha = 0. \end{cases}$

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Interestingly, if we 'rotate' this function by replacing $\frac{k\pi}{n}$ with $\frac{k\pi}{n} + \theta$, where θ is an arbitrary 'angle', it still satisfies (17), although the remainder terms 'hidden' in the $O\left(t^{2n}\right)$ term will change.

In the limit as $n \to \infty$, (17) becomes $G(t) = \int_0^1 g\left(\sin \pi x,\, t\right) dx$. (Rotation now corresponds to shifting the range of integration, which leaves the value of the integral unchanged.) If we apply the substitution $u = \sin \pi x$, we get

$$G(t) = 2\int_0^{1/2} g\left(\sin \pi x,\, t\right) dx = \frac{2}{\pi}\int_0^1 \frac{u \cos ut}{u - \sin ut}\,\frac{du}{\sqrt{1 - u^2}}. \qquad (18)$$

This is valid when $t < 1$ and also generates the series in (16).

And finally …

Returning to my original problem, the probability that my four numbers didn't round correctly to 3, 4 or 5 DP is $(1 - p(3))^3 = \left(1 - \frac{2}{3}\right)^3 \approx 0.037$. (Note that the numbers in my list were constrained to add up to 1, so we need to subtract 1 degree of freedom from the value of n.) So perhaps I was just unlucky with the set of numbers I was working with. Next time I will avoid the whole issue by adding the disclaimer 'Because of rounding, the totals don't necessarily add up exactly.'!

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