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Week 3: Extending the Precision

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Goals

- In the previous week, floating-point arithmetic of precision p was presented.
- We call precision p a *working precision* of a computer (most commonly this is the precision that hardware computes in).
- The main goal this week is to learn of the ways to extend the accuracy of results beyond the working precision.
- There are two strategies of interest:
  1. Use hardware precision p to obtain more accurate results as unevaluated sum of two or more values in precision p.
  2. Use software to compute in higher precision than p.

Literature

The following material, and the references therein, can be used for further reading.

- *Handbook of Floating-Point Arithmetic* by J.-M. Muller and others, 2nd edition, 2018 (HFPA18).
  - Sections 4.3 and 4.4 on `2Sum`, `Fast2Sum` and `2MultFMA` algorithms.
  - Section 5.3 on accurate summation algorithms.
  - Most of Chapter 14.
- Various useful details on summation algorithms are in Chapter 4 of *Accuracy and Stability of Numerical Algorithms* by N. J. Higham, 2nd edition, 2002 (ASNA02).

Contents

- Mixed-precision arithmetic and algorithms.
- `2Sum`, `Fast2Sum`, and `2MultFMA` algorithms.
- Summation algorithms: recursive, compensated, and cascaded summation.
- Arbitrary-precision arithmetic libraries.
- Stochastic rounding: motivation, usage, and advantages in summation.

Some remarks

- As in the previous weeks, we refer to floating point with the abbreviation "FP".
- We refer to FP operations with $\circ\,(a \operatorname{op} b)$ with $\circ \in \{\mathrm{RN}, \mathrm{RZ}, \mathrm{RU}, \mathrm{RD}\}$ and $\operatorname{op} \in \{+, -, \times, /, \sqrt{}\}$.
- We refer to exact operations with $a \operatorname{op} b$.
- We use the *italic* font to emphasize the important terms.
- We use the `typewriter` font for algorithms and code.
- For the multiplication we use `*` in the algorithms and $\times$ in the equations.

Mixed-precision

- Mixed-precision arithmetic can be understood in two ways:
  - ❑ Mixed-precision operations—an adder, a multiplier, or other, that produces an answer by using multiple precisions (internally, or input/output).
  - ❑ Mixed-precision algorithms—algorithms that utilize operations of different (finite) precisions at different steps.
- Note the different terminology used in literature: mixed precision, arbitrary precision, variable precision, multiple precision, infinite precision—the first concept differs from the other four.

Mixed-precision

- An arithmetic operator with the same precision in inputs/outputs is called a *homogeneous* operator.
- An arithmetic operator with different precisions in inputs/outputs is called a *nonhomogeneous* operator.
- Most processors today implement only homogenous arithmetic operations.
- IEEE 754 (1985) did not include a requirement for nonhomogeneous variants.
- Later iterations of the standard include them, but hardware has not yet caught up.

Mixed-precision: FMA

- One example of mixed-precision is the `FMA` instruction, that appears in most modern CPUs (covered briefly last week).
- Given three FP precision-p numbers a, b, and c, the `FMA` instruction computes $\mathrm{RN}(a\times b + c)$.
- Since by definition there can only be one rounding error in the whole computation, the result of $a\times b$ is not rounded before the addition.
- It is held exactly in a wider internal format of $2p$ bits; in this format the addition of c is performed followed by rounding back to p.

Mixed-precision in algorithms

Consider adding 2^{-24} a hundred million times to a variable initialized to 1 in binary32 arithmetic (see example `mixed_precision_example0.c`).

```c
#include <stdio.h>
#include <math.h>

int main() {
  float sum = 1;
  float addend = pow(2, -24);

  for (int i = 1; i < 100000000; i++)
    sum = sum + addend;

  printf("%.30f \n", sum);
}
```

- In this example we do not have any mixed precision.
- All the variables are `float`.
- This basic computation should add the small value a hundred million times to 1 and return ~ 6.96.
- However, it returns 1.
- The problem is that `addend` is too small to be added to 1 in binary32 arithmetic—the sum is rounded to 1 on each iteration.

Mixed-precision in algorithms

We can fix this problem by introducing higher precision in the addition step (see `mixed_precision_example1.c`).

```
1 #include <stdio.h>
2 #include <math.h>
3
4 int main() {
5   float sum = 1;
6   float addend = pow(2, -24);
7
8   double temp_sum = sum;
9
10   for (int i = 1; i < 100000000; i++)
11     temp_sum = temp_sum + addend;
12
13   sum = (float)temp_sum;
14
15   printf("%.30f \n", sum);
16 }
```

- On line 8, we convert `sum` to binary64 precision temporarily.
- On line 11, we perform binary64 addition.
- On line 13 we convert the temporary sum back to binary32 precision.
- The answer produced by this program now is $6.96046 \ldots$
- Both programs produce a binary32 answer, but one produces a completely wrong answer.

Optional exercise

- Modify `mixed_precision_example0.c` to produce the right answer.
- Do not use mixed-precision—only use the binary32 (`float`) variables.
- The exact answer is 6.9604644775390625.
- Once done, compare with the solution in `mixed_precision_example2.c`.

Mixed-precision in algorithms

- But note that the technique showed above can impact performance if binary64 arithmetic is more expensive than binary32 (depends on the processor that is used).
- Other direction that is sometimes taken is to reduce the precision in different parts of a program or algorithm.
- If a computer has fast low-precision arithmetic, find the parts in your algorithms that can leverage it without causing major errors.
- Therefore, mixed-precision algorithms are used either to improve accuracy or performance.
- This kind of programming requires very good knowledge of the underlying hardware.

2Sum and Fast2Sum algorithms

- Given two FP precision-p numbers, a and b, we can obtain s and t such that $s = \mathrm{RN}(a+b)$ and $s + t = a + b$.
- Here s and t are precision-p FP numbers.
- These methods are called *error-free transformations.*
- Note that $\mathrm{RN}(x)$ refers to *round-to-nearest ties-to-even* rounding mode, which is a default mode on most processors.
- Other rounding modes cannot assure the error-free property.
- We can think of s as the answer we get from the FP addition, and t as the rounding error in the addition.
- When a tuple (s, t) represents one quantity, we say that it is represented as an *unevaluated sum* of two floating-point values.
- Note that computing the sum of s and t does not achieve anything, since $\mathrm{RN}(s+t) = s$, so it is only useful to have them separately.

2Sum and Fast2Sum algorithms

```
Algorithm 3.1: Fast2Sum
  inputs a, b, with |a| ≥ |b|
  s  = RN(a + b)
  b' = RN(s - a)
  t  = RN(b - b')
  return (s, t)
```

- Here is one algorithm that performs an error-free transform.
- Note that arguments have to be sorted by magnitude.
- The rounding mode must be RN, otherwise t would not be an *exact error*.

- However, even if the two requirements are violated, the sum of s and t might still be good a approximation to the sum of a and b.
- `Fast2Sum` is useful in *compensated summation* algorithms that take inputs sorted in any way (see later slides).

Fast2Sum informal explanation

```
Algorithm 3.1: Fast2Sum
   inputs a, b, with |a| ≥ |b|
   s  = RN(a + b)
   b' = RN(s - a)
   t  = RN(b - b')
   return (s, t)
```

- First step is to simply add the arguments.
- In that addition, we lose* some part of b to rounding.
- The second step obtains the actual, rounded b, b', that was used in the addition.

- The final step computes the size of a piece of b that was lost in the first step.

* Or add something to b, depending on the rounding direction taken by RN.

2Sum and Fast2Sum algorithms

```
Algorithm 3.2: 2Sum
  inputs a, b
  s  = RN(a + b)
  a' = RN(s - b)
  b' = RN(s − a')
  ea = RN(a − a')
  eb = RN(b − b')
  t  = RN(ea + eb)
  return (s, t)
```

- Here is a more robust version of the previous.
- Advantage over `Fast2Sum` is that no sorting of arguments is required.
- Similar principle, but now either a or b can have smaller magnitude.
- The algorithm does not assume which.
- In steps 2 and 3, either $a' = a$ or $b' = b$.
- Therefore only one of e_a or e_b can be nonzero.
- The algorithm has 2× more steps, but the *depth* is 5—steps 4 and 5 are parallel.

Optional exercise

- Check `2sum.c` in the example code where two `floats` are added with the two presented algorithms.
- Run it and observe the outputs.
- Notice what results `Fast2Sum` computes when arguments are swapped.
- Check that $s \neq a + b$.
- Confirm with more precision (for example, on paper) that we have performed an error-free addition by checking that

$$s + t = a + b.$$

2MultFMA algorithm

```
Algorithm 3.3: 2MultFMA
   inputs a, b
   s  = RN(a * b)
   t  = RN(a * b - s)
   return (s, t)
```

- Now we look at the multiplication.
- This requires the `FMA` instruction (see week 2) for performing the second step.
- First step performs a basic multiplication operation.
- The result from step 1 is a rounded multiplication result.
- In step 2, the FMA is used to compute the multiplication again (but recall that without rounding) and subtract the rounded result.
- Thus, t is the error induced in step 1, and $a \times b = s + t$.
- But there are some exceptions: $t \neq a \times b - s$ for very small a and b (underflow).

Multi-word arithmetic

- There exists algorithms for performing arithmetic operations on numbers that are held as unevaluated sums of multiple FP numbers.
- For example, we may produce two double-precision values from one of the algorithms presented above.
- Then, if we wish to keep computing using those two numbers, we can use *multi-word arithmetic algorithms*.
- Those interested, see the Sec. 14.1 of HFPA18 for more details.

Summation algorithms

- Summation of a series of FP numbers is at the core of scientific computing.
- It is required in, to name a few places, vector products, matrix vector products, matrix-matrix products, means, variances, and polynomial evaluation.
- Accumulation of values as the data is being generated occurs in ODE and PDE solvers, weight updates in machine learning, and similar.
- FP arithmetic can benefit both from changing the order of summands as well as algorithmic approaches that leverage error-free transformations.

Summation algorithms

- Summation involves a problem of adding n values $x_1, \dots, x_n$ in FP arithmetic.
- That is, we wish to compute $\sum_{i=1}^{n} x_i$.
- Naturally, we wish to have the best possible accuracy.
- For simplicity we will deal with nonnegative values $x_i \geq 0$.
- There are many techniques to perform FP summation, but the accuracy depends on the data being summed and there is no best solution generally.
- Those interested in various complex issues with different data distributions and summation, start with Chapter 4 of ASNA02.

Recursive summation

```
Algorithm 3.4: RecSum
  inputs x_1,…,x_n.
  s = x_1
  for i = 2 to n
    s = RN(s + x_i)
  return s
```

- A straightforward solution is to read data in the order it is stored/computed and accumulate it.
- This technique is called *recursive summation*.
- On every iteration we add a relative error of up to $u = 2^{-p}$ due to rounding in the addition operation.

- The order of operations can play an important role in reducing the final error of the computed sum.
- If we sort in decreasing order, then we will be adding increasingly small quantities to an increasingly bigger sum—this can result in more roundoff errors.

Recursive summation

- If we instead sort in an increasing order, we will be adding increasingly large values to an increasingly large sum.
- This usually results in less shifting of the significands and therefore less rounding errors.
- Consider a problem of computing the *harmonic series:*

$$\sum_{i=1}^{\infty} \frac{1}{i} = 1 + \frac{1}{2} + \frac{1}{3} + \dots$$

- This series is known as a *divergent series*, but it is also known to converge to some value in limited precision arithmetics, such as used in computers.
- We modify the problem and compute the truncated series for some number of steps N, that is, we compute $\sum_{i=1}^{N} \frac{1}{N}$.

Recursive summation: harmonic series

- None of the limited-precision arithmetics can compute harmonic series exactly, and all of them can be said to be wrong right from the start.
- However, if we declare that double precision harmonic sum is our *reference solution*, we can compare other arithmetics to it.

```c
#include <stdio.h>
#include <math.h>

int main() {
  float fsum = 0;
  double dsum = 0;
  long int N = 1000000;

  for (int i = 1; i <= N; i++) {
    fsum += (float)1/(float)i;
    dsum += (double)1/(double)i;
  }

  printf("fsum = %.10f, dsum = %.10f, dsum - fsum = %.10f \n",
         fsum, dsum, dsum-fsum);

}
```

- The example code in `recursive_sum0.c` sums the harmonic series for $N = 10^6$ in an increasing order.
- This program produces:

`fsum`	`14.3573579788`
`dsum`	`14.3927267229`
`dsum-fsum`	`0.0353687440`

Recursive summation: harmonic series

- We can reverse the order of evaluation and sum with recursive summation from $i = 10^6$ to $i = 1$, starting from the smallest addend.
- The example code is in `recursive_sum1.c`.

```c
#include <stdio.h>
#include <math.h>

int main() {
  float fsum = 0;
  double dsum = 0;
  long int N = 1000000;

  for (int i = N; i > 0; i--) {
    fsum += (float)1/(float)i;
    dsum += (double)1/(double)i;
  }

  printf("fsum = %.10f, dsum = %.10f, dsum - fsum = %.10f \n",
         fsum, dsum, dsum-fsum);

}
```

fsum	14.3926515579
dsum	14.3927267229
dsum-fsum	0.0000751649

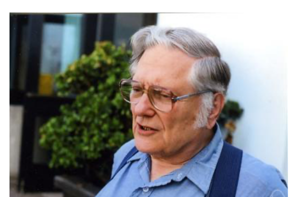
- Notice the change in the computed single precision answer.
- The absolute error is much smaller with the values sorted in an increasing order.

Compensated summation

```
Algorithm 3.5: CompSum
  inputs x_1,…,x_n.
  s = x_1
  t = 0
  for i = 2 to n
    temp = RN(x_i + t)
    (s, t) = Fast2Sum(s, temp)
  end
  return s
```

The algorithm is usually attributed to W. M. Kahan.

Photo: https://en.wikipedia.org/wiki/William_Kahan



- Compensated summation algorithm captures the error in each addition using `Fast2Sum`.
- The key idea is to use the error, induced previously, in the next step.
- If the error is positive (some quantity was removed in rounding), add it.
- If the error is negative (some quantity was added in rounding), then remove it.

Compensated summation: harmonic series

```
12 int main() {
13   float fsum = 0;
14   double dsum = 0;
15   long int N = 1000000;
16   float t = 0;
17
18   for (int i = 1; i <= N; i++) {
19     float addend = (float)1/(float)i + t;
20     fastTwoSum(fsum, addend, &fsum, &t);
21     dsum += (double)1/(double)i;
22   }
23
24   printf("fsum = %.10f, dsum = %.10f, dsum - fsum = %.10f \n",
25          fsum, dsum, dsum-fsum);
26
27 }
```

- Example code in `compensated_sum.c`.
- It further reduces the absolute error.

fsum	14.3927268982
dsum	14.3927267229
dsum-fsum	-0.0000001753

- On line 19, we add the error from the addition in the previous step, to the next element of the series.
- On line 20, we add the sum of them to the overall sum of the series, and compute a new error.

Cascaded summation

```
Algorithm 3.6: CascSum
  inputs x_1,…,x_n.
  s = x_1
  t, e = 0
  for i = 2 to n
    (s, t) = 2Sum(s, x_i)
    e = RN(e + t)
  end
  return RN(s + e)
```

- Here the core idea is to accumulate errors in a separate variable.
- Accumulated errors are added to the total sum at the end.

Cascaded summation: harmonic series

```c
15 int main() {
16   float fsum = 0;
17   double dsum = 0;
18   long int N = 1000000;
19   float t = 0;
20   float e = 0;
21
22   for (int i = 1; i <= N; i++) {
23     float addend = (float)1/(float)i;
24     twoSum(fsum, addend, &fsum, &t);
25     e += t;
26     dsum += (double)1/(double)i;
27   }
28
29   fsum += e;
30
31   printf("fsum = %.10f, dsum = %.10f, dsum - fsum = %.10f \n",
32          fsum, dsum, dsum-fsum);
33
34 }
```

- Example code in `cascaded_sum.c`.
- Worse than compensated summation in this problem.

fsum	14.3927278519
dsum	14.3927267229
dsum-fsum	-0.0000011290

- On line 24, we are adding a new element of the series to the total sum and computing the error of that addition.
- On line 25 we are adding that error into the total sum of errors.
- On line 29, when the series finishes, we add the errors to the sum.

Stagnation

- All the presented summation algorithms are computed in the working precision, but utilize error-free transforms to improve accuracy.
- The main issue with the FP addition is a problem termed *stagnation.*
- It happens when $\mathrm{RN}(a + b) = a$ for some small b.
- Informally, stagnation occurs when the two numbers are so different in magnitude that the operation does not change the larger value.
- b is entirely lost to rounding.
- For example, harmonic series converges due to stagnation, when an addend $\frac{1}{i}$ becomes too small to affect the sum.
- Using mixed-precision or different summation algorithms can help in avoiding stagnation, depending on the problem.

Stagnation

- For single precision arithmetic, stagnation in harmonic series with recursive summation in the decreasing order occurs around $i \approx 2{\times}10^6$.
- Example `stagnation.c` demonstrates this.

```c
#include <stdio.h>
#include <math.h>

int main() {
  float fsum = 0;
  double dsum = 0;
  long int N = 5000000;

  for (int i = 1; i <= N; i++) {
    fsum += (float)1/(float)i;
    dsum += (double)1/(double)i;
    if (i % 1000000 == 0)
      printf("At iteration %d fsum = %.10f, dsum = %.10f \n",
              i, fsum, dsum);
  }

}
```

Stagnation

- Program `stagnation.c` in the examples produces

```
At iteration 1000000 fsum = 14.3573579788, dsum = 14.3927267229
At iteration 2000000 fsum = 15.3110322952, dsum = 15.0858736534
At iteration 3000000 fsum = 15.4036827087, dsum = 15.4913386782
At iteration 4000000 fsum = 15.4036827087, dsum = 15.7790207090
At iteration 5000000 fsum = 15.4036827087, dsum = 16.0021642353
```

- Notice that `fsum` stopped changing sometime after $2\,000\,000$th iteration.
- Double precision continues to add to the overall sum.
- It has been shown in research that double precision stagnates as well after 24 days of run time on a modern processor, after iteration $i = 2^{48}$.

Arbitrary-precision libraries

- One other approach to gain more accurate results is to use arbitrary precision libraries.
- The main principle is that, instead of representing the data in the working precision that the hardware supports, we can represent it in some arbitrary (might be prespecified) precision.
- Arithmetic is performed much slower, and the performance and memory utilization changes with precision.
- May or may not reuse hardware FP arithmetic, or can be based mainly on integer arithmetic.

Arbitrary-precision libraries

Some software and libraries that include arbitrary-precision arithmetics:

- `Mathematica` (general purpose mathematical software),
- `Maple` (software for both numeric and symbolic computing),
- `MATLAB Advanpix toolbox` (provides fast arbitrary precision in MATLAB),
- `MATLAB Symbolic Math Toolbox` (another MATLAB arbitrary precision toolbox), and
- `GNU MPFR` Arbitrary precision library with the interface for C).

Here we use `GNU MPFR` for demonstrating the basic principles.

GNU MPFR basics

- Computations are done on MPFR FP objects which represent numbers or NaN values.
- Each MPFR FP object has its own precision which is specified on initialization of an object.
- MPFR FP objects are similar to IEEE 754 since they have an exponent and a significand, but since this is arbitrary precision, they can occupy multiple registers/memory locations.
- MPFR library provides a wide array of elementary arithmetic operations as well as elementary functions, trigonometric functions, pseudo-random number generators and more, that operate on, and produce, MPFR FP objects.

GNU MPFR example

```
 1 #include <mpfr.h>
 2 #include <stdio.h>
 3
 4 int main (void) {
 5   mpfr_t num, den, res;
 6   mpfr_inits2 (200, num, den, res, (mpfr_ptr) 0);
 7   mpfr_set_si(num, 1, MPFR_RNDN);
 8   mpfr_set_si(den, 3, MPFR_RNDN);
 9
10   mpfr_div(res, num, den, MPFR_RNDN);
11
12   mpfr_printf("1/3 in 200-bit MPFR is %.100Rf \n", res);
13
14   mpfr_clears(num, den, res, (mpfr_ptr) 0);
15
16   double fres = (double)1/3;
17
18   printf("1/3 in double is       %.100f \n", fres);
19 }
```

- The number $1/3 = 0.3333\ldots$ is a *repeating decimal* and cannot be represented in the FP arithmetic.
- We look at what the nearest value is in different computer precisions.
- Example `mpfr_example.c` computes $1/3$ in 200-bit MPFR FP type and double precision.
- Prints out to 100 digits.

- We first include `mpfr.h` on line 1; we then initialize three MPFR type variables (`num, dem, res`) with 200-bit precision (roughly 60 dec. digits) and set `num=1, dem=3` on lines 5–8.
- On lines 10 and 12 we perform MPFR division and print out the result.
- On line 14 we clear the MPFR objects.

GNU MPFR example

```c
#include <mpfr.h>
#include <stdio.h>

int main (void) {
  mpfr_t num, den, res;
  mpfr_inits2 (200, num, den, res, (mpfr_ptr) 0);
  mpfr_set_si(num, 1, MPFR_RNDN);
  mpfr_set_si(den, 3, MPFR_RNDN);

  mpfr_div(res, num, den, MPFR_RNDN);

  mpfr_printf("1/3 in 200-bit MPFR is %.100Rf \n", res);

  mpfr_clears(num, den, res, (mpfr_ptr) 0);

  double fres = (double)1/3;

  printf("1/3 in double is       %.100f \n", fres);
}
```

- The example in `mpfr_example.c` produces the following output.
- The approximations to $1/3$ in 200-bit MPFR FP type and double-precision are shown. As expected, MPFR approximation has more correct digits (more $3's$).

```
192:code_examples mantasmikaitis$ ./mpfr_example
1/3 in 200-bit MPFR is 0.3333333333333333333333333333333333333333333333333333333333334370502546310190284524010675630020706765
1/3 in double is       0.3333333333333333148296162562473909929394721984863281250000000000000000000000000000000000000000000000
```

Stochastic rounding (SR)

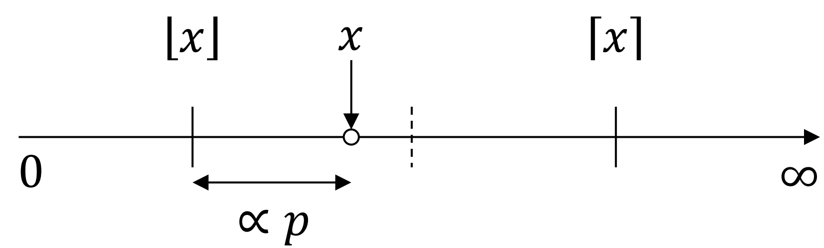
- Some latest hardware for machine learning introduced a rounding mode that does not appear in the IEEE 754 standards.
- It is usually called *stochastic rounding.*
- The main idea of stochastic rounding is to preserve some information of the bits that are thrown away in rounding.
- However, they are not stored explicitly as in error-free transformations, but make impact statistically over multiple roundings.
- Saves memory and hardware costs, since we extend precision without modifying the target precision.
- However, it has expensive rounding logic compared with other rounding modes since *(pseudo)random number generation* is required.

Stochastic rounding (SR)

Given $x \in \mathbb{R}$ with $\lfloor x \rfloor \le x \le \lceil x \rceil$ (when $x \notin F$ it is between the two neighbouring floats), stochastic rounding (SR) is defined as

$$\mathrm{SR}(x) = \begin{cases} \lceil x \rceil & \textbf{with the probability } p, \\ \lfloor x \rfloor & \textbf{with the probability } 1 - p. \end{cases}$$

Mode 1	$p = 0.5$
Mode 2	$p = \dfrac{x - \lfloor x \rfloor}{\mathrm{ulp}(x)}$



Here $\mathbf{ulp}(x)$ is a gap between $\lfloor x \rfloor$ and $\lceil x \rceil$.

With mode 2, $\mathbb{E}\big(\mathrm{SR}(x)\big) = x$.

Stochastic rounding (SR)

- Consider a demonstrative example of computing, in integer arithmetic,

$$0.25 + 0.25 + 0.25 + 0.25 = 1.$$

- Each addend has to be rounded to integer to perform the addition using an integer adder (note, in reality we would use fixed-point arith.).
- With round to nearest, we get

$$\mathrm{RN}(0.25) + \mathrm{RN}(0.25) + \mathrm{RN}(0.25) + \mathrm{RN}(0.25) = 0.$$

- Not an unexpected result since we have to round each 0.25 to the nearest integer, 0.
- With stochastic rounding mode 2 we most likely get

$$\mathrm{SR}(0.25) + \mathrm{SR}(0.25) + \mathrm{SR}(0.25) + \mathrm{SR}(0.25) = 1.$$

- The probability of rounding 0.25 to 1 is $p = \frac{1}{4}$, whereas rounding to 0 it is $1 - p = \frac{3}{4}$. Therefore, one out of 4 roundings above produces 1.

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