# part1

September 4, 2019

## 1 Floating-point arithmetic

As a data analyst, you will be concerned primarily with *numerical programs* in which the bulk of the computational work involves floating-point computation. This notebook guides you through some of the most fundamental concepts in how computers store real numbers, so you can be smarter about your number crunching.

### 1.1 WYSInnWYG, or "what you see is not necessarily what you get."

One important consequence of a binary format is that when you print values in base ten, what you see may not be what you get! For instance, try running the code below.

> This code invokes Python's `decimal` package, which implements base-10 floating-point arithmetic in software.

```
In [1]: from decimal import Decimal
        ?Decimal # Asks for a help page on the Decimal() constructor

In [2]: x = 1.0 + 2.0**(-52)

        print(x)
        print(Decimal(x)) # What does this do?

        print(Decimal(0.1) - Decimal('0.1')) # Why does the output appear as it does?
```

```
1.0000000000000002
1.0000000000000002220446049250313080847263336181640625
5.551115123125782702118158340E-18
```

> Aside: If you ever need true decimal storage with no loss of precision (e.g., an accounting application), turn to the `decimal` package. Just be warned it might be slower. See the following experiment for a practical demonstration.

```
In [3]: from random import random

        NUM_TRIALS = 2500000
```

```
        print("Native arithmetic:")
        A_native = [random() for _ in range(NUM_TRIALS)]
        B_native = [random() for _ in range(NUM_TRIALS)]
        %timeit [a+b for a, b in zip(A_native, B_native)]

        print("\nDecimal package:")
        A_decimal = [Decimal(a) for a in A_native]
        B_decimal = [Decimal(b) for b in B_native]
        %timeit [a+b for a, b in zip(A_decimal, B_decimal)]
```

```
Native arithmetic:
193 ms ś 26.3 ms per loop (mean ś std. dev. of 7 runs, 1 loop each)

Decimal package:
649 ms ś 7.95 ms per loop (mean ś std. dev. of 7 runs, 1 loop each)
```

**The same and not the same.** Consider the following two program fragments:
*Program 1*:

```
s = a - b
t = s + b
```

*Program 2*:

```
s = a + b
t = s - b
```

Let $a = 1.0$ and $b = \epsilon_d/2 \approx 1.11 \times 10^{-16}$, i.e., machine epsilon for IEEE-754 double-precision. Recall that we do not expect these programs to return the same value; let's run some Python code to see.

> Note: The IEEE standard guarantees that given two finite-precision floating-point values, the result of applying any binary operator to them is the same as if the operator were applied in infinite-precision and then rounded back to finite-precision. The precise nature of rounding can be controlled by so-called *rounding modes*; the default rounding mode is "round-half-to-even."

```
In [4]: a = 1.0
        b = 2.**(-53) # == $\epsilon_d$ / 2.0

        s1 =  a - b
        t1 = s1 + b

        s2 =  a + b
        t2 = s2 - b

        print("s1:", s1.hex())
        print("t1:", t1.hex())
```

```
        print("\n")
        print("s2:", s2.hex())
        print("t2:", t2.hex())

        print("")
        print(t1, "vs.", t2)
        print("(t1 == t2) == {}".format(t1 == t2))
```

```
s1: 0x1.fffffffffffffp-1
t1: 0x1.0000000000000p+0


s2: 0x1.0000000000000p+0
t2: 0x1.fffffffffffffp-1

1.0 vs. 0.9999999999999999
(t1 == t2) == False
```

By the way, the NumPy/SciPy package, which we will cover later in the semester, allows you to determine machine epsilon in a portable way. Just note this fact for now.

Here is an example of printing machine epsilon for both single-precision and double-precision values.

```
In [5]: import numpy as np

        EPS_S = np.finfo (np.float32).eps
        EPS_D = np.finfo (float).eps

        print("Single-precision machine epsilon:", float(EPS_S).hex(), "~", EPS_S)
        print("Double-precision machine epsilon:", float(EPS_D).hex(), "~", EPS_D)
```

```
Single-precision machine epsilon: 0x1.0000000000000p-23 ~ 1.1920929e-07
Double-precision machine epsilon: 0x1.0000000000000p-52 ~ 2.220446049250313e-16
```

## 1.2 Analyzing floating-point programs

Let's say someone devises an algorithm to compute $f(x)$. For a given value $x$, let's suppose this algorithm produces the value $\text{alg}(x)$. One important question might be, is that output "good" or "bad?"

**Forward stability.** One way to show that the algorithm is good is to show that

$$|\text{alg}(x) - f(x)|$$

is "small" for all $x$ of interest to your application. What is small depends on context. In any case, if you can show it then you can claim that the algorithm is *forward stable*.

**Backward stability.** Sometimes it is not easy to show forward stability directly. In such cases, you can also try a different technique, which is to show that the algorithm is, instead, *backward stable*.

In particular, $\text{alg}(x)$ is a *backward stable algorithm* to compute $f(x)$ if, for all $x$, there exists a "small" $\Delta x$ such that

$$\text{alg}(x) = f(x + \Delta x).$$

In other words, if you can show that the algorithm produces the exact answer to a slightly different input problem (meaning $\Delta x$ is small, again in a context-dependent sense), then you can claim that the algorithm is backward stable.

**Round-off errors.** You already know that numerical values can only be represented finitely, which introduces round-off error. Thus, at the very least we should hope that a scheme to compute $f(x)$ is as insensitive to round-off errors as possible. In other words, given that there will be round-off errors, if you can prove that $\text{alg}(x)$ is either forward or backward stable, then that will give you some measure of confidence that your algorithm is good.

Here is the "standard model" of round-off error. Start by assuming that every scalar floating-point operation incurs some bounded error. That is, let $a \odot b$ be the exact mathematical result of some operation on the inputs, $a$ and $b$, and let $\text{fl}(a \odot b)$ be the *computed* value, after rounding in finite-precision. The standard model says that

$$\text{fl}(a \odot b) \equiv (a \odot b)(1 + \delta),$$

where $|\delta| \leq \epsilon$, machine epsilon.

Let's apply these concepts on an example.

### 1.3 Example: Computing a sum

Let $x \equiv (x_0, \ldots, x_{n-1})$ be a collection of input data values. Suppose we wish to compute their sum.

The exact mathematical result is

$$f(x) \equiv \sum_{i=0}^{n-1} x_i.$$

Given $x$, let's also denote its exact sum by the synonym $s_{n-1} \equiv f(x)$.

Now consider the following Python program to compute its sum:

```
In [6]: def alg_sum(x): # x == x[:n]
            s = 0.
            for x_i in x: # x_0, x_1, \ldots, x_{n-1}
                s += x_i
            return s
```

In exact arithmetic, meaning without any rounding errors, this program would compute the exact sum. (See also the note below.) However, you know that finite arithmetic means there will be some rounding error after each addition.

Let $\delta_i$ denote the (unknown) error at iteration $i$. Then, assuming the collection `x` represents the input values exactly, you can show that `alg_sum(x)` computes $\hat{s}_{n-1}$ where

$$\hat{s}_{n-1} \approx s_{n-1} + \sum_{i=0}^{n-1} s_i \delta_i,$$

that is, the exact sum *plus* a perturbation, which is the second term (the sum). The question, then, is under what conditions will this sum will be small?

Using a *backward error analysis*, you can show that

$$\hat{s}_{n-1} \approx \sum_{i=0}^{n-1} x_i(1+\Delta_i) = f(x+\Delta),$$

where $\Delta \equiv (\Delta_0, \Delta_1, \ldots, \Delta_{n-1})$. In other words, the computed sum is the exact solution to a slightly different problem, $x + \Delta$.

To complete the analysis, you can at last show that

$$|\Delta_i| \leq (n-i)\epsilon,$$

where $\epsilon$ is machine precision. Thus, as long as $n\epsilon \ll 1$, then the algorithm is backward stable and you should expect the computed result to be close to the true result. Interpreted differently, as long as you are summing $n \ll \frac{1}{\epsilon}$ values, then you needn't worry about the accuracy of the computed result compared to the true result:

```
In [7]: print("Single-precision: 1/epsilon_s ~= {:.1f} million".format(1e-6 / EPS_S))
        print("Double-precision: 1/epsilon_d ~= {:.1f} quadrillion".format(1e-15 / EPS_D))
```

```
Single-precision: 1/epsilon_s ~= 8.4 million
Double-precision: 1/epsilon_d ~= 4.5 quadrillion
```

Based on this result, you can probably surmise why double-precision is usually the default in many languages.

In the case of this summation, we can quantify not just the *backward error* (i.e., $\Delta_i$) but also the *forward error*. In that case, it turns out that

$$|\hat{s}_{n-1} - s_{n-1}| \lessapprox n\epsilon \|x\|_1.$$

**Note: Analysis in exact arithmetic.** We claimed above that `alg_sum()` is correct *in exact arithmetic*, i.e., in the absence of round-off error. You probably have a good sense of that just reading the code.

However, if you wanted to argue about its correctness more formally, you might do so as follows using the technique of proof by induction. When your loops are more complicated and you want to prove that they are correct, you can often adapt this technique to your problem.

First, assume that the `for` loop enumerates each element `p[i]` in order from `i=0` to `n-1`, where `n=len(p)`. That is, assume `p_i` is `p[i]`.

Let $p_k \equiv$ `p`$[k]$ be the $k$-th element of `p[:]`. Let $s_i \equiv \sum_{k=0}^{i} p_k$; in other words, $s_i$ is the *exact* mathematical sum of `p[:i+1]`. Thus, $s_{n-1}$ is the exact sum of `p[:]`.

Let $\hat{s}_{-1}$ denote the initial value of the variable `s`, which is 0. For any $i \geq 0$, let $\hat{s}_i$ denote the *computed* value of the variable `s` immediately after the execution of line 4, where $i =$ `i`. When $i =$ `i` $= 0$, $\hat{s}_0 = \hat{s}_{-1} + p_0 = p_0$, which is the exact sum of `p[:1]`. Thus, $\hat{s}_0 = s_0$.

Now suppose that $\hat{s}_{i-1} = s_{i-1}$. When `i` $= i$, we want to show that $\hat{s}_i = s_i$. After line 4 executes, $\hat{s}_i = \hat{s}_{i-1} + p_i = s_{i-1} + p_i = s_i$. Thus, the computed value $\hat{s}_i$ is the exact sum $s_i$.

If $i = n$, then, at line 5, the value `s` $= \hat{s}_{n-1} = s_{n-1}$, and thus the program must in line 5 return the exact sum.

### 1.4 A numerical experiment: Summation

Let's do an experiment to verify that these bounds hold.

**Exercise 0** (2 points). In the code cell below, we've defined a list,

```
N = [10, 100, 1000, 10000, 100000, 1000000, 10000000]
```

- Take each entry `N[i]` to be a problem size.
- Let `t[:len(N)]` be a list, which will hold computed sums.
- For each `N[i]`, run an experiment where you sum a list of values `x[:N[i]]` using `alg_sum()`. You should initialize `x[:]` so that all elements have the value `0.1`. Store the computed sum in `t[i]`.

```
In [8]: N = [10, 100, 1000, 10000, 100000, 1000000, 10000000]

        # Initialize an array t of size len(N) to all zeroes.
        t = [0.0] * len(N)

        # Your code should do the experiment described above for
        # each problem size N[i], and store the computed sum in t[i].

        ###
        ### YOUR CODE HERE
        ###
        for i in range(0,len(N)):
            t[i]=alg_sum([0.1]*N[i])
        print(t)
```

```
[0.9999999999999999, 9.99999999999998, 99.9999999999986, 1000.0000000001588, 10000.000000018848
```

```
In [9]: # Test: `experiment_results`
        import pandas as pd
        from IPython.display import display

        import matplotlib.pyplot as plt
        %matplotlib inline

        s = [1., 10., 100., 1000., 10000., 100000., 1000000.] # exact sums
        t_minus_s_rel = [(t_i - s_i) / s_i for s_i, t_i in zip (s, t)]
        rel_err_computed = [abs(r) for r in t_minus_s_rel]
        rel_err_bound = [ni*EPS_D for ni in N]

        # Plot of the relative error bound
        plt.loglog (N, rel_err_computed, 'b*', N, rel_err_bound, 'r--')

        print("Relative errors in the computed result:")
        display (pd.DataFrame ({'n': N, 'rel_err': rel_err_computed, 'rel_err_bound': [n*EPS_D
```

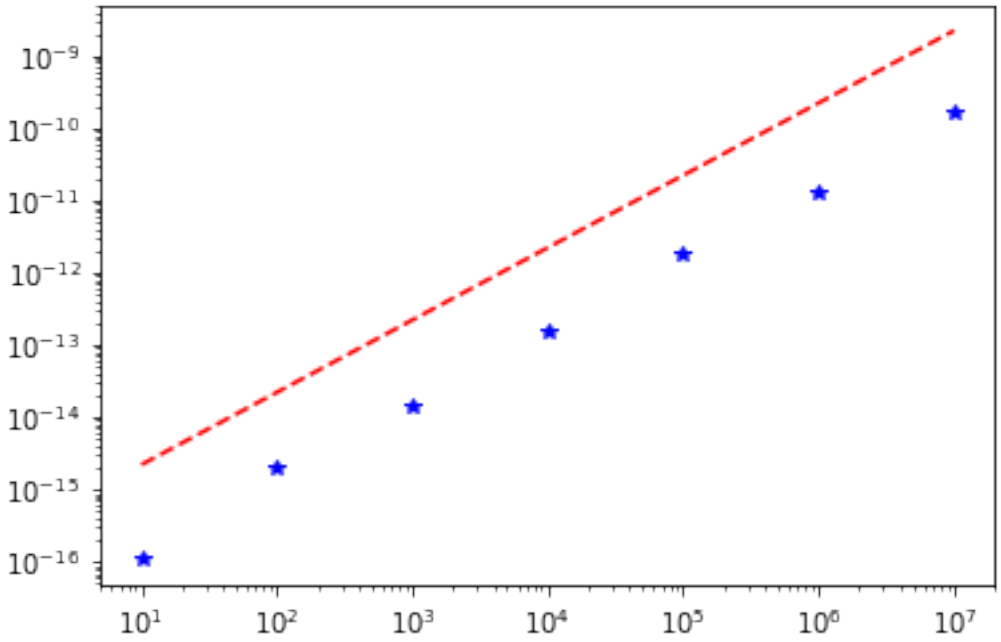
```
        assert all([abs(r) <= n*EPS_D for r, n in zip(t_minus_s_rel, N)])

        print("\n(Passed!)")
```

```
Relative errors in the computed result:


          n       rel_err  rel_err_bound
0        10  1.110223e-16   2.220446e-15
1       100  1.953993e-15   2.220446e-14
2      1000  1.406875e-14   2.220446e-13
3     10000  1.588205e-13   2.220446e-12
4    100000  1.884837e-12   2.220446e-11
5   1000000  1.332883e-11   2.220446e-10
6  10000000  1.610246e-10   2.220446e-09


(Passed!)
```




## 1.5 Computing dot products

Let $x$ and $y$ be two vectors of length $n$, and denote their dot product by $f(x,y) \equiv x^T y$.

Now suppose we store the values of $x$ and $y$ *exactly* in two Python arrays, `x[0:n]` and `y[0:n]`. Further suppose we compute their dot product by the program, `alg_dot()`.