18.335 Problem Set 1 Solutions

Problem 1: (10 points)

The smallest integer that cannot be exactly represented is $n = \beta^t + 1$ (for base-β with a t-digit mantissa). You might be tempted to think that β^t cannot be represented, since a t-digit number, at first glance, only goes up to $\beta^t - 1$ (e.g. three base-10 digits can only represent up to 999, not 1000). However, β^t can be represented by $\beta^{t-1} \cdot \beta^1$, where the β^1 is absorbed in the exponent.

In IEEE single and double precision, $\beta = 2$ and $t = 24$ and 53, respectively, giving $2^{24} + 1 =$ 16,777,217 and $2^{53} + 1 =$ 9,007,199,254,740,993.

Evidence that $n = 2^{53} + 1$ is not exactly represented but that numbers less than that are can be presented in a variety of ways. In the pset1-solutions notebook, we check exactness by comparing to Julia's `Int64` (built-in integer) type, which exactly represents values up to $2^{63} - 1$.

Problem 2: (10+10 points)

See the pset1 solutions notebook for Julia code, results, and explanations.

Problem 3: (10+10+10 points)

(a) We will exploit the Taylor expansions of f and f' around the root x_*

$$f(x_* + \delta) = \cancel{f(x_*)} + \underbrace{f'(x_*)}_{f'_*}\delta + \underbrace{f''(x_*)}_{f''_*}\frac{\delta^2}{2} + O(\delta^3),$$
$$f'(x_* + \delta) = f'_* + f''_*\delta + O(\delta^2).$$

The Newton step $\delta_{n+1} = \delta_n - f(x_n)/f'(x_n)$ can then be expanded in δ_n as

$$\begin{aligned}\delta_{n+1} &= \delta_n - \frac{f'_* + f''_*\frac{\delta_n}{2} + O(\delta_n^2)}{f'_*\left[1 + \frac{f''_*}{f'_*}\delta_n + O(\delta_n^2)\right]}\delta_n = \\ &= \delta_n - \left(1 + \frac{f''_*}{f'_*}\delta_n\right)\left[1 - \frac{f''_*}{2f'_*}\delta_n\right]\delta_n + O(\delta_n^3) \\ &= \boxed{+\frac{f''_*}{2f'_*}\delta_n^2} + O(\delta_n^3)\end{aligned}$$

as desired, assuming $f'_* \neq 0$. Note that we used the fact that $\frac{1}{1+u} = 1 - u + O(u^2)$ (another Taylor expansion!) to move the denominatory into the numerator, and we are sweeping all of the higher-order terms into $O(\delta_n^3)$.

(b) See the pset1 solutions notebook for Julia code, results, and explanations.

(c) See the pset1 solutions notebook for Julia code, results, and explanations.

Problem 4: (10+5+10 points)

Here you will analyze $f(x) = \sum_{i=1}^n x_i$ as in class, but this time you will compute $\tilde{f}(x)$ in a different way. In particular, compute $\tilde{f}(x)$ by a recursive divide-and-conquer approach known in the literature

as **pairwise summation**, recursively dividing the set of values to be summed in two halves and then summing the halves:

$$\tilde{f}(x) = \begin{cases} 0 & \text{if } n = 0 \\ x_1 & \text{if } n = 1 \\ \tilde{f}(x_{1:\lfloor n/2 \rfloor}) \oplus \tilde{f}(x_{\lfloor n/2 \rfloor + 1:n}) & \text{if } n > 1 \end{cases},$$

where $\lfloor y \rfloor$ denotes the greatest integer $\leq y$ (i.e. y rounded down). In exact arithmetic, this computes $f(x)$ exactly, but in floating-point arithmetic this will have very different error characteristics than the simple sequential summation in class.

(a) Suppose $n = 2^m$ with $m \geq 1$. We will first show that

$$\tilde{f}(x) = \sum_{i=1}^{n} x_i \prod_{k=1}^{m} (1 + \epsilon_{i,k})$$

where $|\epsilon_{i,k}| \leq \epsilon_{\text{machine}}$. We prove the above relationship by induction. For $n = 2$ it follows from the definition of floating-point arithmetic. Now, suppose it is true for n and we wish to prove it for $2n$. The sum of $2n$ number is first summing the two halves recursively (which has the above bound for each half since they are of length n) and then adding the two sums, for a total result of

$$\tilde{f}(x \in \mathbb{R}^{2n}) = \left[\sum_{i=1}^{n} x_i \prod_{k=1}^{m} (1 + \epsilon_{i,k}) + \sum_{i=n+1}^{2n} x_i \prod_{k=1}^{m} (1 + \epsilon_{i,k}) \right] (1 + \epsilon)$$

for $|\epsilon| < \epsilon_{\text{machine}}$. The result follows by inspection, with $\epsilon_{i,m+1} = \epsilon$.

Then, we use the result from class that $\prod_{k=1}^{m}(1 + \epsilon_{i,k}) = 1 + \delta_i$ with $|\delta_i| \leq m\epsilon_{\text{machine}} + O(\epsilon^2_{\text{machine}})$. Since $m = \log_2(n)$, the desired result follows immediately.

(b) Just enlarge the base case. Instead of recursively dividing the problem in two until $n < 2$, divide the problem in two until $n < N$ for some N, at which point we sum the $< N$ numbers with a simple loop as in problem 2. A little arithmetic reveals that this produces $\sim 2n/N$ function calls—this is negligible compared to the $n - 1$ additions required as long as N is sufficiently large (say, $N = 200$), and the efficiency should be roughly that of a simple loop. (See the pset1 Julia notebook for benchmarks and explanations.)

Using a simple loop has error bounds that grow as N as you showed above, but N is just a constant, so this doesn't change the overall logarithmic nature of the error growth with n. A more careful analysis analogous to above reveals that the worst-case error grows as $[N + \log_2(n/N)]\epsilon_{\text{machine}} \sum_i |x_i|$. Asymptotically, this is not only $\log_2(n)\epsilon_{\text{machine}} \sum_i |x_i|$ error growth, but with the same asymptotic constant factor (same coefficient of the $\log_2 n$ term)!

(c) Instead of "if (n < 2)," just do (for example) "if (n < 200)". See the notebook for code and results.

The basic problem here is that recursion has a small overhead, and if the base case is $n < 2$ then the overhead is significant compared to the trivial computation of the base case. You can try to make recursion cheaper (e.g. trying to beat the compiler by managing a manual stack), but there is no way to bring the cost down to that of a trivial base case. Instead, the simplest thing to do is to make the base case more expensive by stopping at a larger n and switching to a naive loop. This is also called "recursion coarsening."

There are also a few other tricks, basically in making the base-case loop faster: enabling SIMD instructions (in Julia with "@simd") and turning off array bounds-checking, for example.