18.335 Midterm Solutions, Fall 2012

Problem 1: (25 points)

Note that your solutions in this problem don't require you to know how sin, ln, and Γ are calculated on a computer, because the answers rely on properties of the *functions* (and of floating-point arithmetic in general, of course), not of the algorithms to compute the functions. (Contrary to what many students assumed, Taylor series are *not* the only way to compute special functions like this, nor are they usually the best way except in limiting cases, nor should you generally use the *same* Taylor series for all x.)

(a) The condition number of $f(x) = \sin(x)$ is $\kappa(x) = \frac{f'(x)}{f(x)/x} = x \frac{\cos x}{\sin x}$. As $x \to 0$, $\kappa(x) \to 1$ (since $\frac{\sin x}{x} \to 1$), so it is well conditioned near x = 0 and we should expect an accurate answer is possible even if there is a small (relative) rounding error in x. In particular, the Taylor expansion of $\sin x$ near x = 0 clearly becomes more and more accurate as $x \to 0$, in which limit $\sin x \approx x$ and the function f(x) = x can obviously be computed accurately (with the forward error approaching the relative error in x). On the other hand, $x \to 2\pi$, $\frac{\sin x}{x} \to 0$ and hence $\kappa(x) \to \infty$: the problem is ill-conditioned near 2π and a small forward error may not be possible, depending upon how we define the problem.

In particular, if x contains a small relative error, e.g. because it was rounded from a non-representable real number, then we should not expect a small forward error near 2π : the large condition number means that a small error in x produces a large error in $\sin x$. For example, for $x = 2\pi + \delta$ with $\delta \sim \varepsilon_{\text{machine}}$, a roundoff error to $\tilde{x} = 2\pi + \delta + \varepsilon_{\text{machine}}$ will roughly double the magnitude of $\sin(x)$, giving a relative error of order 1.

If the input x is exactly computed in floating point, on the other hand then it is possible to compute an accurate answer. Suppose that we computed $\sin(x)$ near $x=2\pi$ by first computing $y=x-2\pi$ and then computing $\sin y$. If we naively computed y by y=x $\operatorname{fl}(2\pi)$, we could easily get a large cancellation error in computing y since 2π is not exactly representable. However, if we instead computed $\operatorname{fl}(x-2\pi)=(x-2\pi)[1+O(\varepsilon_{\operatorname{machine}})]$, e.g. by performing the subtraction in a higher precision, then we could obtain a small forward error in $\sin y=\sin x$.

(b) For $|x| < \varepsilon_{\text{machine}}$, 1+x will be rounded to 1 and hence $\log(1+x)$ would give 0 (a relative error of 1 for $x \neq 0$!). Therefore, we need a specialzed $\log 1p(x)$ function if we wish to compute $\ln(1+x)$ accurately for small |x|.

Equivalently, the function $\ln(y)$ has a condition number $\frac{1/y}{\ln(y)/y}$ that diverges as $y \to 1$, making it extraordinarily sensitive to rounding errors in computing the argument y = 1 + x, while the function $f(x) = \ln(1+x)$ has condition number $\frac{1/(1+x)}{\ln(1+x)/x} \to 1$ as $x \to 0$.

A possible implementation might use the Taylor expansion $\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + O(x^5)$ for small x, and compute $\ln(1+x)$ directly for larger x. e.g.

$$\log 1p(x) = \begin{cases} x \left(1 - x \left(\frac{1}{2} - x \left(\frac{1}{3} - \frac{x}{4}\right)\right)\right) & |x| < 10^{-3} \\ \log(1 + x) & \text{otherwise} \end{cases},$$

(where for extra niceness I evaluated $x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4}$ by Horner's method). This four-term Taylor series should be accurate to machine precision for $|x| < 10^{-3}$.

[The problem is *not* points near (slightly bigger than) x = -1. If you want to compute $\ln(1+x)$ for such x, there is no way around the fact that you need to know 1+x accurately to know how close the argument of the log is to zero, and cancellation errors will force you to lose a lot of significant digits in finding 1+x if x is not exactly representable. A specialized log1p function won't help. Note also

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that if fl(x) > -1, we will obtain $1 \oplus x > 0$ in exactly rounded floating-point arithmetic, so rounding won't change the domain of the function.]

(c) The problem in this case is not roundoff errors, but overflow. Remember that floating-point uses a fixed number of digits for its exponent, so it cannot represent arbitrarily large numbers. (In double precision, the maximum magnitude is $\approx 10^{308}$). The factorial function, and hence the $\Gamma(x)$ function, grows faster than exponentially with x, so for $x \gtrsim 172$ it will overflow and simply give ∞ . By defining a separate gammaln(x) function, Matlab allows you to study the magnitude of the Γ function for much larger x (up to $x \approx 10^{305}$).

Note that, if it weren't for overflow, there wouldn't necessarily be any severe accuracy problem with computing $\ln \Gamma(x)$ by computing $\Gamma(x)$ first. $\ln(x)$ is well-conditioned for large x. The condition number of $\Gamma(x)$ does grow with x, but only relatively slowly ($\approx x \ln x$), so it overflows long before it becomes badly conditioned.

Problem 2: (5+10+10 points)

- (a) A simple example would be $||(x,y)||_+ = ||x|| + ||y||$. Another would be $||(x,y)||_{max} = \max(||x||, ||y||)$. More examples are $||(x,y)||_p = \sqrt[p]{||x||^p + ||y||^p}$ for any $p \ge 1$. All of these clearly satisfy the positivity, scaling, and triangle properties of norms, inheriting those properties from the norms on x and y (combined with the same properties of the L_p norm).
- (b) Second \Longrightarrow First, but not the other way around. That is, the Second definition is a stronger requirement on \tilde{f} . [Note that, from class, equivalence of norms means that we only need to prove this for one choice of $\|(x,y)\|$ and it follows for all other choices of norm.]

Suppose that \tilde{f} is backwards stable in the Second sense. Then, using e.g. $\|(x,y)\|_{\max}$ from above, we have $\|\tilde{x}-x\|=\|x\|O(\varepsilon_{\text{machine}}) \leq \|(x,y)\|_{\max}O(\varepsilon_{\text{machine}})$ and $\|\tilde{y}-y\|=\|y\|O(\varepsilon_{\text{machine}}) \leq \|(x,y)\|_{\max}O(\varepsilon_{\text{machine}})$. Hence $\|(\tilde{x},\tilde{y})-(x,y)\|_{\max}=\max(\|\tilde{x}-x\|,\|\tilde{y}-y\|)=\|(x,y)\|_{\max}O(\varepsilon_{\text{machine}})$, and First follows.

The converse is not true, essentially because we can have $\|x\|$ arbitrarily small compared to $\|(x,y)\|$ by choosing $\|x\| \ll \|y\|$ (or vice versa). From $\|\tilde{x} - x\| \le \|(\tilde{x}, \tilde{y}) - (x, y)\|_{\max} = \|(x, y)\|O(\varepsilon_{\text{machine}})$, we obtain $\|\tilde{x} - x\| = \frac{\|(x,y)\|}{\|x\|} \|x\|O(\varepsilon_{\text{machine}})$. However, it does not follow that $\|\tilde{x} - x\| = \|x\|O(\varepsilon_{\text{machine}})$, because the prefactor $\frac{\|(x,y)\|}{\|x\|}$ can be arbitrarily large, and we required the constants in $O(\varepsilon_{\text{machine}})$ to be independent of x (uniform convergence).

More explicitly, let us construct a counterexample (not required). Consider $f(x,A) = bx^* + A$ for $x \in \mathbb{C}^n$, $A \in \mathbb{C}^{n \times n}$, and some fixed $b \in \mathbb{C}^n$. It is straightforward to show that this is backwards-stable in the First sense, by letting $\tilde{x} = x$ and $\tilde{A} = \tilde{f}(x,A) - bx^*$. i.e. $\tilde{A}_{ij} = (b_i \otimes x_j \oplus A_{ij}) - b_i x_j = [b_i x_j (1+\varepsilon_1) + A_{ij}](1+\varepsilon_2) - b_i x_j = A_{ij} + b_i x_j [\varepsilon_1 + O(\varepsilon_{\text{machine}}^2)] + A_{ij} \varepsilon_2$, where $|\varepsilon_{1,2}| \leq \varepsilon_{\text{machine}}$. Hence $|\tilde{A}_{ij} - A_{ij}| \leq (\|x\|_{\infty} + \|A\|_{\infty})O(\varepsilon_{\text{machine}})$ (where $\|A\|_{\infty} = \max_{i,j} |A_{ij}|$) and we have $\|\tilde{A} - A\|_{\infty} = \|(x,A)\|_{+}O(\varepsilon_{\text{machine}})$. Hence it is backwards stable in the First sense. On the other hand, it is not backwards stable in the Second sense. Consider inputs A = 0, in which case $f(\tilde{x},A)$ is rank 1 for any \tilde{x} , but $\tilde{f}(x,A)$ will not be rank 1 due to roundoff errors [similar to pset 2 problem 4(b)(ii)], and hence

we must have $\tilde{A} \neq A$ in order to have $f(\tilde{x}, \tilde{A}) = \tilde{f}(x, A)$. But then $||\tilde{A} - \tilde{A}|| = ||\tilde{A}|| > ||\tilde{A}|| = 0$ and therefore it cannot satisfy the Second definition.

(c) Choose $\|(x,y)\| = \|x\|_1 + \|y\|_1$, in which case both the norm and the algorithm $\tilde{f}(x,y)$ are exactly equivalent to the summation studied and proved backwards stable in class, applied to a column vector $\begin{pmatrix} x \\ y \end{pmatrix} \in \mathbb{R}^{m+n}$. So, it is stable in the First sense.

In fact, it is stable in the Second sense as well! Since it is stable in the First sense, construct (\tilde{x}, \tilde{y}) with $f(\tilde{x}, \tilde{y}) = \tilde{f}(x, y)$ and $\|(\tilde{x}, \tilde{y}) - (x, y)\|_{\infty} = \|(x, y)\|_{\infty} O(\varepsilon_{\text{machine}})$ for $\|(x, y)\|_{\infty} = \max(\|x\|_{\infty}, \|y\|_{\infty})$. Suppose $\|x\|_{\infty} \geq \|y\|_{\infty}$, then it follows that $\|\tilde{x} - x\|_{\infty} \leq \|(\tilde{x}, \tilde{y}) - (x, y)\|_{\infty} = \|x\|_{\infty} O(\varepsilon_{\text{machine}})$, and we only need to prove the corresponding property for $\tilde{y} - y$, but unfortunately this is not true if $\|y\|_{\infty} \ll \|x\|_{\infty}$. Instead, let us construct a new pair (\tilde{x}', \tilde{y}') with $f(\tilde{x}', \tilde{y}') = f(\tilde{x}, \tilde{y}) = \tilde{f}(x, y)$ by setting $\tilde{y}' = y$, and $\tilde{x}_i' = \tilde{x}_i + \frac{\sum (\tilde{y}_k - y_k)}{m}$ for $i = 1, \dots, m$ —that is, we have pushed all of the $\tilde{y} - y$ differences into \tilde{x}' , while keeping the sum the same. Then $\|\tilde{y}' - y\| = 0 = \|y\|O(\varepsilon_{\text{machine}})$ and $\|\tilde{x}' - x\|_{\infty} \leq \|\tilde{x} - x\|_{\infty} + \|\tilde{y} - y\|_{\infty} \leq 2\|(\tilde{x}, \tilde{y}) - (x, y)\|_{\infty} = \|x\|_{\infty} O(\varepsilon_{\text{machine}})$. Similarly if $\|x\|_{\infty} \leq \|y\|_{\infty}$, except that we push all the $\tilde{x} - x$ differences into \tilde{y}' . Hence it is backwards stable in the Second sense.

You could also use the analysis from pset 2 (or similar) to explicitly construct \tilde{x} and \tilde{y} and thereby prove stability in the Second (hence First) sense.

Problem 3: (25 points)

First, let us follow the hint and show that $q_k = Q^{(n)}e_k$ is in the span $\langle x_1, x_2, \dots, x_k \rangle$ as $n \to \infty$. We will proceed by induction on k. Let

$$v_k = A^n e_k = \sum_{i=1}^m c_i \lambda_i^n x_i,$$

where we have expanded $e_k = \sum c_i x_i$ in the basis of the eigenvectors; we can generically assume that $c_i \neq 0$ for all i, so that v_k is dominated as $n \to \infty$ by the terms with the biggest $|\lambda|$.

- For k = 1, $q_1 = v_1/\|v_1\|_2$ (via Gram-Schmidt), and since $v_1 \approx c_1 \lambda_1^n x_1$ as $n \to \infty$ we have $q_1 \to x_1$.
- Suppose $q_i \in \langle x_1, \dots, x_i \rangle$ for i < k, and prove for k. For large n,

$$v_k \approx \sum_{i \leq k} c_i \lambda_i^n x_i \in \langle x_1, \dots, x_k \rangle,$$

where we have discarded the i > k terms as negligible. We obtain q_k from v_k by Gram-Schmidt:

$$q_k = \frac{v_k - \sum_{i < k} q_i q_i^* v_k}{\| \cdots \|_2}.$$

However, since all of the terms in the numerator are $\in \langle x_1, \dots, x_k \rangle$, the result follows. (Note that the orthonormality of the q's means that q_k must contain a nonnegligible x_k component, as otherwise it would be in the span of the q_i for i < k.)

It is instructive (but not strictly necessary!) to look at this more carefully. Since the q_i for i < k, being independent, necessarily form a *basis* for the (k-1) subspace $\langle x_1, \ldots, x_{k-1} \rangle$, it follows that $(I - \sum_{i < k} q_i q_i^*) x_j = 0$ for j < k (since we are projecting orthogonal to the whole $\langle x_1, \ldots, x_k \rangle$ subspace). Hence,

$$q_k pprox \frac{c_k \mathcal{X}_k^{r}[x_k - \sum_{i < k} q_i q_i^* x_k]}{\| \cdots \|_2} \in \langle x_1, \dots, x_k \rangle.$$

So, like in class, q_k still picks up contributions only from the λ_k^n term in v_k , as all of the larger $|\lambda|$ terms are cancelled by the projection. (At least, in exact arithmetic, but fortunately the QR iteration gives us the same result without the ill-conditioning.) Unlike the Hermitian case in class, however, $q_i^* x_k \neq 0$ in general, so q_k generally has nonzero x_i components for i < k.

Now that we have proven this fact, the result is easy. Since $q_k \in \langle x_1, \dots, x_k \rangle$, it immediately follows that $Aq_k \in \langle x_1, \dots, x_k \rangle = \langle q_1, \dots, q_k \rangle$, and thus $T_{ij} = q_i^* A q_k = 0$ for i > k. Hence $T = Q^* A Q$ is upper triangular, and we have a Schur factorization of A.

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18.335J Introduction to Numerical Methods Spring 2019

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