### 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 $\Gamma$ 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 $\kappa(x)=\frac{f^{\prime}(x)}{f(x) / x}=x \frac{\cos x}{\sin x}$. As $x \rightarrow 0, \kappa(x) \rightarrow 1$ (since $\frac{\sin x}{x} \rightarrow 1$ ), 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 $x \rightarrow 0$, 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, $x \rightarrow 2 \pi, \frac{\sin x}{x} \rightarrow 0$ and hence $\kappa(x) \rightarrow \infty$ : the problem is ill-conditioned near $2 \pi$ 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 $2 \pi$ : 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 $y=x \quad \mathrm{fl}(2 \pi)$, we could easily get a large cancellation error in computing $y$ since $2 \pi$ is not exactly representable. However, if we instead computed $\mathrm{fl}(x-2 \pi)=(x-2 \pi)\left[1+O\left(\varepsilon_{\text {machine }}\right)\right]$, 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 $\log (1+\mathrm{x})$ would give 0 (a relative error of 1 for $x \neq 0$ !). Therefore, we need a specialzed $\log 1 \mathrm{p}(\mathrm{x})$ 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 $y \rightarrow 1$, 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 $\frac{1 /(1+x)}{\ln (1+x) / x} \rightarrow 1$ as $x \rightarrow 0$.

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

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

(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 $\log 1 \mathrm{p}$ function won't help. Note also
that if $\mathrm{fl}(x)>-1$, 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 $\infty$. By defining a separate gammaln(x) function, Matlab allows you to study the magnitude of the $\Gamma$ 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 $p \geq 1$. 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. $\|(x, y)\|_{\text {max }}$ from above, we have $\|\tilde{x}-x\|=\|x\| O\left(\varepsilon_{\text {machine }}\right) \leq\|(x, y)\|_{\max } O\left(\varepsilon_{\text {machine }}\right)$ and $\|\tilde{y}-y\|=\|y\| O\left(\varepsilon_{\text {machine }}\right) \leq$ $\|(x, y)\|_{\max } O\left(\varepsilon_{\text {machine }}\right)$. Hence $\|(\tilde{x}, \tilde{y})-(x, y)\|_{\max }=\max (\|\tilde{x}-x\|,\|\tilde{y}-y\|)=\|(x, y)\|_{\max } O\left(\varepsilon_{\text {machine }}\right)$, 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 $\|\tilde{x}-x\| \leq\|(\tilde{x}, \tilde{y})-(x, y)\|_{\max }=\|(x, y)\| O\left(\varepsilon_{\text {machine }}\right)$, we obtain $\|\tilde{x}-x\|=\frac{\|(x, y)\|}{\|x\|}\|x\| O\left(\varepsilon_{\text {machine }}\right)$. However, it does not follow that $\|\tilde{x}-x\|=\|x\| O\left(\varepsilon_{\text {machine }}\right)$, 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 $f(x, A)=b x^{*}+A$ 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 backwardsstable in the First sense, by letting $\tilde{x}=x$ and $\tilde{A}=\tilde{f}(x, A)-b x^{*}$. i.e. $\tilde{A}_{i j}=\left(b_{i} \otimes x_{j} \oplus A_{i j}\right)-b_{i} x_{j}=$ $\left[b_{i} x_{j}\left(1+\varepsilon_{1}\right)+A_{i j}\right]\left(1+\varepsilon_{2}\right)-b_{i} x_{j}=A_{i j}+b_{i} x_{j}\left[\varepsilon_{1}+O\left(\varepsilon_{\text {machine }}^{2}\right)\right]+A_{i j} \varepsilon_{2}$, where $\left|\varepsilon_{1,2}\right| \leq \varepsilon_{\text {machine }}$. Hence $\left|\tilde{A}_{i j}-A_{i j}\right| \leq\left(\|x\|_{\infty}+\|A\|_{\infty}\right) O\left(\varepsilon_{\text {machine }}\right)$ (where $\|A\|_{\infty}=\max _{i, j}\left|A_{i j}\right|$ ) and we have $\|\tilde{A}-A\|_{\infty}=$ $\|(x, A)\|_{+} O\left(\varepsilon_{\text {machine }}\right)$. 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 $\left\|\tilde{A}-A^{0}\right\|^{0}=\|\tilde{A}\|>\Downarrow A \|_{O}^{0}\left(\varepsilon_{\text {machine }}\right)$, 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 $\binom{x}{y} \in \mathbb{R}^{m+n}$. 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 $\|(\tilde{x}, \tilde{y})-(x, y)\|_{\infty}=\|(x, y)\|_{\infty} O\left(\varepsilon_{\text {machine }}\right)$ for $\|(x, y)\|_{\infty}=\max \left(\|x\|_{\infty},\|y\|_{\infty}\right)$. Suppose $\|x\|_{\infty} \geq\|y\|_{\infty}$, then it follows that $\|\tilde{x}-x\|_{\infty} \leq\|(\tilde{x}, \tilde{y})-(x, y)\|_{\infty}=\|x\|_{\infty} O\left(\varepsilon_{\text {machine }}\right)$, 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 $\left(\tilde{x}^{\prime}, \tilde{y}^{\prime}\right)$ with $f\left(\tilde{x}^{\prime}, \tilde{y}^{\prime}\right)=f(\tilde{x}, \tilde{y})=\tilde{f}(x, y)$ by setting $\tilde{y}^{\prime}=y$, and $\tilde{x}_{i}^{\prime}=\tilde{x}_{i}+\frac{\sum\left(\tilde{y}_{k}-y_{k}\right)}{m}$ for $i=1, \ldots, m$-that is, we have pushed all of the $\tilde{y}-y$ differences into $\tilde{x}^{\prime}$, while keeping the sum the same. Then $\left\|\tilde{y}^{\prime}-y\right\|=0=\|y\| O\left(\varepsilon_{\text {machine }}\right)$ and $\left\|\tilde{x}^{\prime}-x\right\|_{\infty} \leq$ $\|\tilde{x}-x\|_{\infty}+\frac{\sum\left(\tilde{y}_{k}-y_{k}\right)}{m} \leq\|\tilde{x}-x\|_{\infty}+\|\tilde{y}-y\|_{\infty} \leq 2\|(\tilde{x}, \tilde{y})-(x, y)\|_{\infty}=\|x\|_{\infty} O$ ( $\varepsilon_{\text {machine }}$ ). Similarly if $\|x\|_{\infty} \leq\|y\|_{\infty}$, except that we push all the $\tilde{x}-x$ differences into $\tilde{y}^{\prime}$. 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 $\left\langle x_{1}, x_{2}, \ldots, x_{k}\right\rangle$ as $n \rightarrow \infty$. 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 $n \rightarrow \infty$ by the terms with the biggest $|\lambda|$.

- For $k=1, q_{1}=v_{1} /\left\|v_{1}\right\|_{2}$ (via Gram-Schmidt), and since $v_{1} \approx c_{1} \lambda_{1}^{n} x_{1}$ as $n \rightarrow \infty$ we have $q_{1} \rightarrow x_{1}$.
- Suppose $q_{i} \in\left\langle x_{1}, \ldots, x_{i}\right\rangle$ for $i<k$, and prove for $k$. For large $n$,

$$
v_{k} \approx \sum_{i \leq k} c_{i} \lambda_{i}^{n} x_{i} \in\left\langle x_{1}, \ldots, x_{k}\right\rangle
$$

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 $\in\left\langle x_{1}, \ldots, x_{k}\right\rangle$, 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 $\left\langle x_{1}, \ldots, x_{k-1}\right\rangle$, it follows that $\left(I-\sum_{i<k} q_{i} q_{i}^{*}\right) x_{j}=0$ for $j<k$ (since we are projecting orthogonal to the whole $\left\langle x_{1}, \ldots, x_{k}\right\rangle$ subspace). Hence,

$$
q_{k} \approx \frac{c_{k} \lambda_{k}^{\pi}\left[x_{k}-\sum_{i<k} q_{i} q_{i}^{*} x_{k}\right]}{\|\cdots\|_{2}} \in\left\langle x_{1}, \ldots, x_{k}\right\rangle
$$

So, like in class, $q_{k}$ still picks up contributions only from the $\lambda_{k}^{n}$ 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 $q_{k} \in\left\langle x_{1}, \ldots, x_{k}\right\rangle$, it immediately follows that $A q_{k} \in\left\langle x_{1}, \ldots, x_{k}\right\rangle=\left\langle q_{1}, \ldots q_{k}\right\rangle$, and thus $T_{i j}=q_{i}^{*} A q_{k}=0$ for $i>k$. Hence $T=Q^{*} A Q$ is upper triangular, and we have a Schur factorization of $A$.

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