Beyond machine precision: high-accuracy computation of Chebyshev coefficients in floating point arithmetic

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Chebyshev polynomials and corresponding polynomial expansions have so many desirable properties for numerical purposes that it is easy to be happy with what we have. Indeed, many computations can be performed up to machine precision accuracy with fast algorithms and that seems impossible to improve upon. Yet, at least for analytic functions, there is reason to doubt whether that is the case.

The computation of Chebyshev coefficients using the discrete cosine transform yields very small absolute errors, on the order of machine precision if the function is known with sufficient accuracy. However, the late coefficients in the expansion are very small and their relative error with this standard algorithm is $\mathcal{O}(1)$. In this talk we point out that an alternative computation of Chebyshev coefficients, for analytic functions, via contour integrals in the complex plane yields a relative error on the order of machine precision. This implies that the late coefficients are also computed with full precision. One can even compute coefficients that are smaller than machine precision, with 15 accurate digits. In some cases the computations can still be performed efficiently with the FFT. The contour integral approach is very much related to the accurate computation of high-order derivatives of analytic functions using Cauchy integrals, as recently described by Bornemann.

Of course one can not approximate a function with less than machine precision absolute error. One advantage of having more accurate small coefficients is that no accuracy is lost after differentiation, since this loss of accuracy is due to large relative errors. This implies potential improved accuracy in rootfinding, in particular rootfinding on derivatives of a function. We can show fully numerically using Chebyshev expansions that the 100th-order derivative of the exponential function is still the exponential function, to 15 digits, using just floating point accuracy computations.