MY PAPERS ON NUMERICAL MATHEMATICS

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Introduction.

I worked from 1959 to 1985 as a reactor physicist at the research establishment Risø. As part of my work I devised methods for numerical solution of various equations. In particular two problem areas were of interest: rootfinding and solution of the neutron diffusion equation.

Rootfinding.

The problem to solve is the following:

Let the real function f be calculable in the closed interval $I = [a, b]$, and assume that $f(a)$ and $f(b)$ have opposite signs. Find two points c and d in I, such that $f(c)$ and $f(d)$ have opposite signs, and $|c - d| < \epsilon$, where ϵ is a preassigned positive real number.

In the sixties I constructed a lot of algorithms to solve this problem. The first really successful one was HYP, described in [1]. At that time the usual algorithms used polynomial approximations to f when estimating the root. But as soon as the degree of the approximating polynomial is greater than 1, the formulae become complicated. I found that simpler formulae resulted if one let the approximating rational function have real singularities, and the practical difficulties connected with avoiding singularities in the interval $[a, b]$ were surmountable. Actually, [1] is my only success when it comes to number of quotations.

In [2] I gave a general account of methods using rational approximation to f and described (20 years after the first version appeared!) a particular (and very complicated) high order method HYPAR which had proved itself close to optimal for a particular problem in reactor physics.

In 1965 I also described (in an internal report) a method where, in place of the function f, one considered the inverse function f^{-1}. Here the problem reduces to finding the value assumed at the particular point 0. The formulae are simpler, even for arbitrary degree of the approximating polynomial. However, I did not succeed in constructing a competitive algorithm using this method, so I did not publish it.

I later found that there was nothing new in the mathematics connected with these methods. One sometimes forgets that before the advent of programmable calculating machines one was even more dependent on efficient numerical methods.

The neutron diffusion equation.

The density n of neutrons in a nuclear reactor is governed by the neutron transport equation. A reasonable approximation is obtained by simplifying the dependence of n on the direction of flight. In this way we arrive at the neutron diffusion equation for the neutron flux ϕ. To simplify the dependence of ϕ on energy we divide the energy interval into a finite number of energy groups. For each group

the dependence on the properties (the neutron cross sections) of the material is averaged over energy.

It turns out that we get a system of coupled elliptic partial differential equations for the group fluxes. Actually we have an eigenvalue problem, in which the fission terms are provided with a factor λ, the eigenvalue determining the distance of the reactor from criticality. There are usually infinitely many eigenvalues, but the one we are interested in is the smallest positive eigenvalue. When trying to increase the speed of the calculations one often assumes that all eigenvalues are positive. I proved already in 1960 (see [3] and the supplementary notes in [6]) that this assumption is not always justified. However, in some cases it is, and one must assume that in most practical cases the eigenvalues cluster around the positive part of the real axis so that the acceleration methods work satisfactorily.

These remarks are relevant when using the methods of solution developed during the fifties, where the number of neutron groups was rather small (the two group approximation was widely used). The iterations needed to arrive from an initial guess (usually a spacewise constant flux) to the flux corresponding to the smallest positive eigenvalue λ were called outer iterations.

But each outer iteration required that one should solve each group equation for the neutron energy group to which it corresponded, considering the contributions from the other groups as source terms. This was done iteratively, the inner iterations.

Later on, it was found by numerical experimentation that one could simplify this iterative method considerably, with a corresponding gain in speed. One can say that the outer iteration was simplified by performing only one inner iteration in each group. Apparently the success of the method depended critically on the way in which a new guess for the eigenvalue was arrived at at the end of an outer iteration. The one actually used consisted in simply adding all equations and solving the resulting linear equation for λ.

I showed in [4] that this method did not always work. However, it was difficult to find cases of failure for the method, and these cases were rather exotic. I showed in [5], that a different way of calculating λ actually could be proven to work in a number of cases, for instance in one group theory. But a simple iterative method of this type, working in all cases, seemed to be non-existing.

References

1. G. K. Kristiansen, *Zero of arbitrary function*, BIT (Nordisk tidsskrift for informationsbehandling) **3** (1963), 205–206.
2. _____, *A rootfinder using a nonmonotone rational approximation*, SIAM J. Sci. Stat. Comput. **6** (1985), 118–127.
3. _____, *Description of DC-2, a two-dimensional, cylindrical geometry, two-group diffusion theory code for DASK, and a discussion of the theory for such codes*, RisøReport no. 55, Danish atomic energy commission research establishment Risø, 1963.
4. _____, *The convergence of the equipoise method*, Nucl. Sci. Eng. **16** (1963), 133–134.
5. _____, *An iterative method for determination of a minimal eigenvalue*, Nucl. Sci. Eng. **31** (1968), 540–541.
6. _____, *On the one-dimensional multi-group diffusion equations*, This website (2010), 1–5.