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Lecture 3. Rootfinding, optimization, and quadrature

1. Rootfinding [*ATAP* chap 18]

To find roots of a function f on an interval, we approximate f by a polynomial "proxy" p and find the roots of p. This idea originates with Jack "007" Good (who also invented "the singularity") in 1961. Its big proponents in recent years have been the Chebfun project and John Boyd, author of *Solving Transcendental Equations: The Chebyshev Polynomial Proxy and Other Numerical Rootfinders, Perturbation Series, and Oracles*, SIAM 2014.

If p has degree less than a few hundred, we compute its roots as eigenvalues of the associated *colleague matrix*. If the degree is higher, we recursively subdivide the interval so that the overall complexity is $O(n^2)$, not $O(n^3)$.

Theorem 18.1. Polynomial roots and colleague matrix eigenvalues. *The roots of the polynomial*

$$p(x) = \sum_{k=0}^{n} a_k T_k(x), \quad a_n \neq 0,$$

are the eigenvalues of the matrix

$$C = \begin{pmatrix} 0 & 1 & & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & & \\ & \frac{1}{2} & 0 & \frac{1}{2} & & \\ & & \ddots & \ddots & \ddots & \\ & & & & & \frac{1}{2} \\ & & & & \frac{1}{2} & 0 \end{pmatrix} - \frac{1}{2a_n} \begin{pmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ a_0 & a_1 & a_2 & \dots & a_{n-1} \end{pmatrix}. \qquad (18.1)$$

(Entries not displayed are zero.) If there are multiple roots, these correspond to eigenvalues with the same multiplicities.

The numbers ½ above are the coefficients of the 3-term recurrence relation for Chebyshev polyonmials. For other orthogonal polynomials, such as Legendre (see below) the matrix has the same structure but different coefficients. (The general case is called a *comrade matrix.*

2. Optimization

Optimization means minimization (or maximization) and is one of the big areas of numerical analysis/scientific computing (others include linear algebra and PDEs). Its importance keeps growing. Key concepts include unconstrained vs constrained, linear vs nonlinear, convex vs nonconvex, 1D vs medium-D vs high-D, local vs global.

In Chebfun, optimization is global, taking advantage of the global polynomial representation of a function. Ultimately this is possible because eigenvalues of matrices are computed globally — "all of them". That in turn is done because the properties of the QR algorithm make computing all eigenvalues quite efficient.

3. Quadrature [*ATAP* chap 19]

A 1D quadrature formula is an approx. such as $I_n = \sum_{k=0}^{n} w_k f(x_k) \approx I = \int_{-1}^{1} f(x)dx$, with *nodes* x_k and *weights* w_k .

Usually the weights are chosen so that I_n is the integral of the degree n polynomial interpolant through $f(x_0), \dots, f(x_n)$.

Chebyshev points: *Clenshaw-Curtis quadrature* (1960). Roots of Legendre polynomials: *Gauss quadrature* (1814).
There's not much difference between C-C and Gauss in practice and <u>*both converge exponentially as $n \to \infty$ if f is analytic*</u>.

Equispaced points: *Newton-Cotes quadrature.* Very bad for large n . Diverges as $n \to \infty$ in general, even if f is analytic, because of the Runge phenomenon. (This was proved by Pólya in 1933.)

Golub-Welsch algorithm for computing nodes and wts (1969): eigenvalue problem as above, with lower coefficients all = 0.

Much faster $O(n)$algorithms discovered in recent years by Bogaert, Hale, Townsend,… implemented in Chebfun `legpts`.