Lecture 16: From Lanczos to Gauss quadrature

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1. Orthogonal polynomials

- Replace $\mathbb{C}^n$ by $L^2[-1,1]$, a vector space of real-valued functions on $[-1,1]$. The inner product of two functions $u, v \in L^2[-1,1]$ is defined by

$$\langle u, v\rangle = \int_{-1}^{1} u(x)v(x)\mathrm{d}x,$$

and the norm of a function $u \in L^2[-1,1]$ is $\|u\| = \langle u, u\rangle^{1/2}$.

Proposition 1

The pointwise multiplication operator $(\mathbf{A}u)(x) = xu(x)$ is self-adjoint with respect to the given inner product.

Proof. Note that

$$\langle \mathbf{A}u, v\rangle = \int_{-1}^{1} (\mathbf{A}u)(x)v(x)\mathrm{d}x = \int_{-1}^{1} u(x)(\mathbf{A}v)(x)\mathrm{d}x = \langle u, \mathbf{A}v\rangle. \qquad \square$$

- The Lanczos process ($\mathbf{r} = 1$ and $\mathbf{A} = x$) becomes the procedure for constructing orthogonal polynomials via a three-term recurrence relation.

Algorithm: Lanczos for orthogonal polynomials

$\beta_0 = 0,\ q_0(x) = 0,\ q_1(x) = 1/\sqrt{2}$

for $j = 1, 2, 3, \ldots,$

  $v(x) = xq_j(x)$

  $\alpha_j = \langle v, q_j \rangle$

  $v(x) = v(x) - \beta_{j-1}q_{j-1}(x) - \alpha_j q_j(x)$

  $\beta_j = \|v\|$

  $q_{j+1}(x) = v(x)/\beta_j$

end

Remark 2

We have $\langle q_i, q_j \rangle = \int_{-1}^{1} q_i(x)q_j(x)\mathrm{d}x = \delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$

Remark 3

The function $q_{j+1}(x)$ *is a scalar multiple of the usual* j*th Legendre polynomial* $P_j(x)$ *of degree* j *(note that* $P_j(1) = 1$*), i.e.,*

$$q_{j+1}(x) = q_{j+1}(1)P_j(x).$$

Remark 4

The three-term recurrence takes the form

$$xq_j(x) = \beta_{j-1}q_{j-1}(x) + \alpha_j q_j(x) + \beta_j q_{j+1}(x).$$

The entries $\{\alpha_j\}$ *and* $\{\beta_j\}$ *are known analytically:*

$$\alpha_j = 0, \qquad \beta_j = \frac{1}{2}(1 - (2j)^{-2})^{-1/2}.$$

- The tridiagonal matrices $\{\mathbf{T}_j\}$ in Lanczos process are known as *Jacobi matrices* in the context of orthogonal polynomials.

Remark 5

If the inner product is modified by the inclusion of a nonconstant positive weight function $w(x)$ in the integrand, then one obtains other families of orthogonal polynomials such as Chebyshev polynomials and Jacobi polynomials.

1.1. Comparison to Gram–Schmidt

Algorithm: Gram–Schmidt for orthogonal polynomials

for $j = 1, 2, 3, \cdots$
  $q_j(x) = x^{j-1}$
  for $i = 1$ **to** $j - 1$
    $r_{ij} = \langle x^{j-1}, q_i \rangle$
    $q_j(x) = q_j(x) - r_{ij} q_i(x)$
  end
  $r_{jj} = \|q_j\|$
  $q_j(x) = q_j(x)/r_{jj}$
end

Remark 6

The above algorithm constructs the continuous QR *factorizations of the "Krylov matrix"*

$$\mathbf{K}_\infty = \left[\begin{array}{ccccc} 1 & x & x^2 & x^3 & \cdots \end{array}\right],$$

which is obtained by setting $\mathbf{r} = 1$ *and* $\mathbf{A} = x$.

Remark 7

The two algorithms obtain the same sequence of functions $\{q_j\}$.

2. Orthogonal polynomials approximation problem

- Find a monic polynomial p^j of degree j such that

$$\|p^j(x)\| = \min_{\text{monic } p,\ \deg(p)=j} \|p(x)\|.$$

The solution is the characteristic polynomial of the matrix $\mathbf{T}_j$.

Theorem 8

Let $p^j(x)$ be the characteristic polynomial of $\mathbf{T}_j$. Then for $j = 0, 1, \cdots$,

$$p^j(x) = \rho_j q_{j+1}(x),$$

where ρ_j is a constant.

Proof. Any monic $p(x)$ of degree j can be written as

$$p(x) = \rho_j q_{j+1}(x) + \sum_{i=1}^{j} y_i q_i(x),$$

where ρ_j is a constant – the inverse of the leading coefficient of $q_{j+1}(x)$. Due to

$$\|p(x)\| = (\rho_j^2 + \|\mathbf{y}\|_2^2)^{1/2},$$

the minimum is obtained by setting $\mathbf{y} = \mathbf{0}$. □

Corollary 9

The zeros of $q_{j+1}(x)$ are the eigenvalues of $\mathbf{T}_j$. These j zeros are distinct and lie in the open interval $(-1,1)$.

Proof. All eigenvalues of $\mathbf{T}_j$ are distinct. Assume that $k < j$. For any $\{x_i\}_{i=1}^k$, we have

$$\int_{-1}^{1} q_{j+1}(x)\mathrm{d}x = 0, \quad \int_{-1}^{1} q_{j+1}(x)\prod_{i=1}^{k}(x - x_i)\mathrm{d}x = 0.$$

The first equality shows that there exists at least one root in $(-1,1)$. Now assume there are only $k < j$ distinct roots in $(-1,1)$, denoted by $\{x_i\}_{i=1}^k$. Consider the polynomial $q_{j+1}(x)\prod_{i=1}^{k}(x - x_i)$, which has constant sign in $(-1,1)$. This is a contradiction of the second equality. □

3. Gauss–Legendre quadrature

- Numerical quadrature: consider a j-point quadrature formula

$$I_j(f) = \sum_{i=1}^{j} w_i f(x_i) \quad \text{for} \quad I(f) = \int_{-1}^{1} f(x)\mathrm{d}x.$$

Theorem 10

Let the nodes $\{x_i\}_{i=1}^{j}$ be an arbitrary set of j distinct points in $[-1,1]$. Then there is a unique choice of wights $\{w_i\}_{i=1}^{j}$ with the property that the quadrature formula has order of accuracy at least $j-1$ in the sense that it is exact if $f(x)$ is any polynomial of degree $\leq j-1$. The weights $\{w_i\}_{i=1}^{j}$ are given by

$$w_i = \int_{-1}^{1} \ell_i(x)\mathrm{d}x, \quad \ell_i(x) = \prod_{k=1,k\neq i}^{j} (x - x_k) \Big/ \prod_{k=1,k\neq i}^{j} (x_i - x_k).$$

- Gauss–Legendre quadrature: $\{x_i\}_{i=1}^{j}$ are the zeros of $q_{j+1}(x)$.

Theorem 11

The j-point Gauss–Legendre quadrature formula has order of accuracy exactly $2j-1$, and no quadrature formula has order of accuracy higher than this.

Proof. Consider the polynomial

$$f(x) = \prod_{i=1}^{j} (x - x_i)^2, \qquad I(f) = \int_{-1}^{1} f(x)\mathrm{d}x > 0.$$

Note that $I_j(f) = 0$ since $f(x_i) = 0$. Thus the quadrature formula has order of accuracy $\le 2j-1$. Suppose $f(x) \in \mathbb{P}_{2j-1}$. Then $f(x)$ can be factored in the form

$$f(x) = g(x) q_{j+1}(x) + r(x),$$

where $g(x) \in \mathbb{P}_{j-1}$ and $r(x) \in \mathbb{P}_{j-1}$. (In fact, $r(x)$ is the unique polynomial interpolant to $f(x)$ in the points $\{x_i\}$.)

Since $q_{j+1}(x)$ is orthogonal to all polynomials of lower degree, we have

$$I(gq_{j+1}) = 0.$$

At the same time, since

$$g(x_i)q_{j+1}(x_i) = 0$$

for each x_i, we have

$$I_j(gq_{j+1}) = 0.$$

Since I and I_j are linear operators, these identities impliy

$$I(f) = I(r) \quad \text{and} \quad I_j(f) = I_j(r).$$

Therefore,

$$I(f) = I_j(f). \quad \square$$

Theorem 12

Let $\mathbf{T}_j$ *be the* $j \times j$ *Jacobi matrix. Let* $\mathbf{T}_j = \mathbf{V}\mathbf{D}\mathbf{V}^\top$ *be an orthogonal diagonalization of* $\mathbf{T}_j$ *with*

$$\mathbf{D} = \mathrm{diag}\{\lambda_1, \cdots, \lambda_j\}, \quad \mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \cdots & \mathbf{v}_j \end{bmatrix}.$$

Then the nodes and weights of the Gauss–Legendre quadrature formula are given by

$$x_i = \lambda_i, \quad w_i = 2(\mathbf{v}_i)_1^2, \quad i = 1, \cdots, j.$$

- G. H. Golub and J. H. Welsch

  Calculation of Gauss quadrature rules, Math. Comp. 23 (1969).

  The famous $O(j^2)$ algorithm for Gauss quadrature nodes and weights via a tridiagonal Jacobi matrix eigenvalue problem.
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