

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

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

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

Proposition 1

The linear operator $\mathbf{A} : L^2[-1, 1] \rightarrow L^2[-1, 1]$ defined by

$$(\mathbf{A}u)(x) = xu(x)$$

is self-adjoint with respect to the given inner product.

Proof. Note that

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

- The Lanczos process ($\mathbf{r} = 1$ and $\mathbf{A} = x$) becomes the procedure for constructing orthogonal polynomials via a three-term recurrence relation: $x [q_1(x) \quad \cdots \quad q_j(x)] = [q_1(x) \quad \cdots \quad q_{j+1}(x)] \tilde{\mathbf{T}}_j$.
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Algorithm: Lanczos process for orthogonal polynomials

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

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

$$v(x) = xq_j(x)$$

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

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

$$v(x) = v(x) - \alpha_j q_j(x)$$

$$\beta_j = \|v\|$$

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

end

$$\tilde{\mathbf{T}}_j = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \ddots & \\ \ddots & \ddots & \ddots & \beta_{j-1} \\ & & \beta_{j-1} & \alpha_j \\ & & & \beta_j \end{bmatrix}$$

Remark 2

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

Remark 3

The function $q_j(x)$ is a scalar multiple of the Legendre polynomial $P_j(x)$ of degree $j - 1$ (note that $P_j(1) = 1$), i.e.,

$$q_j(x) = q_j(1)P_j(x).$$

Remark 4

The three-term recurrence takes the form

$$xq_j(x) = \beta_{j-1}q_{j-1}(x) + \alpha_jq_j(x) + \beta_jq_{j+1}(x).$$

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

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

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

1.1. Comparison to Gram–Schmidt

Algorithm: Gram–Schmidt for orthogonal polynomials

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for  $j = 1, 2, 3, \dots$ 
     $q_j(x) = x^{j-1}$ 
    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
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Remark 5

The above algorithm constructs the continuous QR factorizations of the “Krylov matrix”

$$\mathbf{K}_\infty = [1 \quad x \quad x^2 \quad x^3 \quad \dots],$$

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

Remark 6

The Lanczos and Gram–Schmidt processes both obtain the same sequence of orthogonal polynomials $\{q_j\}$.

Remark 7

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.

2. Orthogonal polynomials approximation problem

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

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

According to Theorem 6 of Lecture 15, the unique solution is the characteristic polynomial of the matrix \mathbf{T}_j .

Theorem 8

For $j = 1, 2, \dots$, the unique solution of the orthogonal polynomials approximation problem is

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

where ρ_j is the inverse of the leading coefficient of $q_{j+1}(x)$.

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 distinct and lie in the open interval $(-1, 1)$.

Proof. From Theorem 6 of Lecture 15 and the last theorem, we know $\rho_j q_{j+1}(x)$ is the characteristic polynomial of \mathbf{T}_j . It follows from all eigenvalues of \mathbf{T}_j are distinct and real that the zeros of $q_{j+1}(x)$ are distinct and real.

Now assume there are only $k < j$ distinct zeros in $(-1, 1)$, denoted by $\{x_i\}_{i=1}^k$. Consider the polynomial

$$q_{j+1}(x) \prod_{i=1}^k (x - x_i) = c(x) \prod_{i=1}^k (x - x_i)^2, \quad c(x) \in \mathbb{P}_{j-k},$$

which has constant sign in $(-1, 1)$. This contradicts the following equality

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

3. Gauss–Legendre quadrature

- A j -point numerical quadrature formula:

$$\mathcal{I}_j(f) = \sum_{i=1}^j w_i f(x_i), \quad x_i \in (-1, 1), \quad \text{for } \mathcal{I}(f) = \int_{-1}^1 f(x) dx.$$

- We call $\mathcal{I}_j(f)$ has order of accuracy exactly m if

$$\mathcal{I}(p) - \mathcal{I}_j(p) = 0, \quad \forall p \in \mathbb{P}_m,$$

and there exists at least one polynomial $p \in \mathbb{P}_{m+1}$ such that

$$\mathcal{I}(p) - \mathcal{I}_j(p) \neq 0.$$

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

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

Theorem 10

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

Proof. For any numerical quadrature formula $\mathcal{I}_j(f) = \sum_{i=1}^j w_i f(x_i)$, consider the polynomial

$$p(x) = \prod_{i=1}^j (x - x_i)^2 \in \mathbb{P}_{2j}.$$

Obviously, we have $\mathcal{I}_j(p) = 0$ and $\mathcal{I}(p) > 0$. Thus the quadrature formula has order of accuracy $\leq 2j - 1$.

Now consider the j -point Gauss–Legendre quadrature. For any $p(x) \in \mathbb{P}_{2j-1}$, it can be factored in the form

$$p(x) = g(x)q_{j+1}(x) + r(x), \quad g(x) \in \mathbb{P}_{j-1}, \quad r(x) \in \mathbb{P}_{j-1}.$$

In fact, $r(x)$ is the unique interpolating polynomial to $p(x)$ in the points $\{x_i\}$ (the zeros of $q_{j+1}(x)$), i.e.,

$$r(x) = \sum_{i=1}^j p(x_i) \ell_i(x).$$

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

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

It follows that

$$\mathcal{I}(p) = \mathcal{I}(gq_{j+1} + r) = \mathcal{I}(gq_{j+1}) + \mathcal{I}(r) = \mathcal{I}(r).$$

Therefore, by

$$\mathcal{I}(r) = \int_{-1}^1 \sum_{i=1}^j p(x_i) \ell_i(x) dx = \sum_{i=1}^j w_i p(x_i) = \mathcal{I}_j(p),$$

we have

$$\mathcal{I}(p) = \mathcal{I}_j(p). \quad \square$$

Theorem 11

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

$$\mathbf{D} = \text{diag}\{\lambda_1, \dots, \lambda_j\}, \quad \mathbf{V} = [\mathbf{v}_1 \ \dots \ \mathbf{v}_j].$$

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

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

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

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

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

- G. H. Golub and G. Meurant

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