

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

*Proof.* Note that

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

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

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**Algorithm:** Lanczos for orthogonal polynomials

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

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

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

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

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

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

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

**end**

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## 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  $q_{j+1}(x)$  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*

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

*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 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

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**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  $j - 1$ 
         $r_{ij} = \langle q_i, x^{j-1} \rangle$ 
         $q_j(x) = q_j(x) - r_{ij}q_i(x)$ 
    end
     $r_{jj} = \|q_j\|$ 
     $q_j(x) = q_j(x)/r_{jj}$ 
end
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## Remark 6

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

$$\mathbf{K}_\infty = \begin{bmatrix} 1 & x & x^2 & x^3 & \cdots \end{bmatrix},$$

*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  $j = 0, 1, \dots$ ,

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

where  $\rho_j$  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  $\rho_j$  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

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

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

- The Gauss–Legendre quadrature formula is defined as the quadrature formula

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

whose nodes  $x_1, \dots, x_j$  are the zeros of  $q_{j+1}(x)$ , and weights  $w_1, \dots, w_j$  are the unique choice with the property that the quadrature has order of accuracy at least  $j - 1$  in the sense that it is exact if  $f(x)$  is any polynomial of degree  $\leq j - 1$ .

- Note that

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

## Theorem 10

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

*Proof.* Consider the polynomial

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

Note that  $I_j(f) = 0$  since  $f(x_i) = 0$ . Thus the quadrature formula has order of accuracy  $\leq 2j - 1$ . 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 degree  $j - 1$  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 imply

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

Therefore,

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

## 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

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

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

- G. H. Golub and G. Meurant

Matrices, Moments and Quadrature with Applications

Princeton University Press, 2010