# Lecture 16: From Lanczos to Gauss quadrature



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## 1. The discrete vector/continuous function analogy

• If discrete vectors become continuous functions on [-1,1] (analogous to column vectors of dimension  $\infty \times 1$ ), and the matrix **A** is taken to be the operator of pointwise multiplication by x, i.e.,

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

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

• The nodes and weights of Gauss quadrature formulas can be computed by solving a symmetric tridiagonal matrix eigenvalue problem.

## 2. 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

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

## **Algorithm**: Lanczos for orthogonal polynomials

$$\beta_0 = 0, \ q_0(x) = 0, \ q_1(x) = 1/\sqrt{2}$$
 for  $j = 1, 2, 3, \dots$ , 
$$v(x) = xq_j(x)$$
 
$$\alpha_j = \langle q_j, v \rangle$$
 
$$v(x) = v(x) - \beta_{j-1}q_{j-1}(x) - \alpha_j q_j(x)$$
 
$$\beta_j = ||v||$$
 
$$q_{j+1}(x) = v(x)/\beta_j$$
 end

### Remark 2

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

#### Remark 3

The function  $q_{j+1}(x)$  is a scalar multiple of the usual jth 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.

## **Algorithm**: Gram–Schmidt for orthogonal polynomials

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

$$q_{j}(x) = x^{j-1}$$
for  $i = 1$  to  $j - 1$ 

$$r_{ij} = \langle q_{i}, x^{j-1} \rangle$$

$$q_{j}(x) = q_{j}(x) - r_{ij}q_{i}(x)$$
end
$$r_{jj} = ||q_{j}||$$

$$q_{j}(x) = q_{j}(x)/r_{jj}$$
end

#### Remark 6

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

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

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

#### Remark 7

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

## 3. 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  $\rho_i$  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 y = 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.

## 4. Gauss-Legendre quadrature

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

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

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

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

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  $I_i$  are linear operators, these identities impliy

$$I(f) = I(r)$$
 and  $I_j(f) = I_j(r)$ .

Therefore,

$$I(f) = I_i(f)$$
.  $\square$ 

#### 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

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

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

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

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