THE UNIVERSITY OF RHODE ISLAND

Gaussian Quadrature & Tridiagonal Matrices

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Introduction

1. Introduce Quadrature Rules.
2. Generalize this to *Gaussian* Quadrature rules.
3. Illustrate some examples.
4. Introduce the tridiagonal matrix eigenvalue problem.

Next time:

1. How can the weights from Gaussian Quadrature be used for other linear algebra algorithms?
2. Lanczos algorithm, Ritz Values & Vectors , . . .

Problem Statement

Goal: Given a function $f \in C[a,b]$, distinct $\{x_0, x_1, \ldots, x_n\} \subset [a,b]$, and $\{w_0, w_1, \ldots, w_n\} \in \mathbb{R}$, we wish to write

$$\int_a^b f(x)\,dx \quad \approx \quad \sum_{j=0}^{n} w_j f(x_j).$$

Motivation:

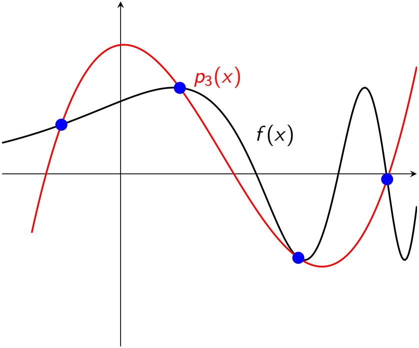
- Perhaps we only know f by its action on some points.
- There may not be an elementary antiderivative of f.

Introduction

Our discussion will be based on interpolary quadrature methods.

Find the n^{th} degree polynomial interpolant p_n to f at the nodes $x_0, \ldots, x_n$.

$$\int_a^b f(x)\,dx \quad \approx \quad \int_a^b p_n(x)\,dx.$$



If $f \in C^{n+1}[a,b]$, the error is

$$\frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x-x_i)f^{(n+1)}(\xi(x))\,dx$$

Constructing $p_n(x)$

Here and going forward, we let

$$\mathcal{P}_n \quad = \quad \{\text{polynomials of degree at most } n\}.$$

Given $n+1$ distinct points $\{x_0, \ldots, x_n\} \subset [a, b]$, the Lagrange basis for $\mathcal{P}_n$ is

$$\{\ell_0, \ell_1, \ldots, \ell_n\}, \quad \text{where} \quad \ell_j(x) = \prod_{\substack{k=0 \\ k \neq j}}^{n} \frac{x - x_k}{x_j - x_k}.$$

Then we have the unique degree n polynomial interpolant to f:

$$p_n(x) = \sum_{j=0}^{n} f(x_j)\ell_j(x)$$

Determining Weights

Now, notice that

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \int_a^b p_n(x)\,dx \\ &= \int_a^b \sum_{j=0}^{n} f(x_j)\ell_j(x)\,dx \\ &= \sum_{j=0}^{n} f(x_j)\int_a^b \ell_j(x)\,dx\end{aligned}$$

Let $w_j = \int_a^b \ell_j(x)\,dx$ for $j = 0, \ldots, n$. Then

$$\int_a^b f(x)\,dx \approx \sum_{j=0}^{n} w_j f(x_j).$$

Quadrature Rule

$$\int_a^b f(x)\,dx \quad \approx \quad \sum_{j=0}^{n} w_j f(x_j), \qquad w_j = \int_a^b \ell_j(x)\,dx \tag{1}$$

Note: When $f \in \mathcal{P}_n$, we have equality.

Definition 1 (Degree of Exactness)

The quadrature rule (1) is said to have *degree of exactness* m if it exactly integrates all polynomials in $\mathcal{P}_m$.

So the $n+1$ point quadrature rule (1) has degree of exactness n.

We will raise the degree of exactness in a clever way.

Generalization of the Problem

To increase the degree of exactness, we consider a generalized problem:

$$\int_a^b f(x)w(x)\,dx \quad \approx \quad \sum_{j=0}^{n} w_j f(x_j)$$

for a weight function $w(x) \in C[a,b]$ and $w(x) \geq 0$ on $[a,b]$.

$$\begin{aligned}
\int_a^b f(x)w(x)\,dx \quad &\approx \quad \int_a^b p_n(x)w(x)\,dx \\
&= \quad \int_a^b \sum_{j=0}^{n} f(x_j)\ell_j(x)w(x)\,dx \\
&= \quad \sum_{j=0}^{n} f(x_j) \int_a^b \ell_j(x)w(x)\,dx \\
&= \quad \sum_{j=0}^{n} w_j f(x_j)
\end{aligned}$$

where $w_j = \int_a^b \ell_j(x)w(x)\,dx$.

Generalization of the Problem

This yields the following generalized $n+1$ point quadrature rule:

$$\int_a^b f(x)w(x)\,dx \quad \approx \quad \sum_{j=0}^{n} f(x_j)w_j \qquad \text{where} \quad w_j = \int_a^b \ell_j(x)w(x)\,dx \qquad (2)$$

(Still has degree of exactness n)

Choosing the nodes x_j and weights w_j in a clever way, we can dramatically increase the degree of exactness of (2) for any $w(x)$.

To do so, we need to use orthogonal polynomials.

Orthogonal Polynomials

As before, consider a weight function $w(x) \in C[a,b]$ where $w(x) \geq 0$ and $w(x) \neq 0$ on any subinterval of $[a,b]$.

Definition 2 (Orthogonal Polynomials)

A set of polynomials $\{\phi_0, \ldots, \phi_{n+1}\}$ (where $\deg(\phi_k) = k$) is said to be an orthogonal set of polynomials with respect to the weight function $w(x)$ if

$$\langle \phi_i(x), \phi_j(x) \rangle := \int_a^b \phi_i(x)\phi_j(x)w(x)\,dx = 0 \qquad \forall\, i \neq j.$$

Orthonormal polynomials (i.e., $\langle \phi_i, \phi_i \rangle = 1$) are not necessary here.

We will now show that the $n+1$ point generalized quadrature rule has degree of exactness $2n+1$.

Generalized Rule Degree of Exactness $2n+1$

Let p be degree $2n+1$ and $\{\phi_0, \ldots, \phi_{n+1}\}$ a set of orthogonal polynomials. Then there exists $q, \ r \in \mathcal{P}_n$ such that

$$p(x) = \phi_{n+1}(x)q(x) + r(x).$$

Then

$$\begin{aligned}
\int_a^b p(x)w(x)\,dx &= \int_a^b \phi_{n+1}(x)q(x)w(x)\,dx + \int_a^b r(x)w(x)\,dx \\
&= \langle \phi_{n+1}(x), q(x) \rangle + \int_a^b r(x)w(x)\,dx \\
&= \left\langle \phi_{n+1}(x), \sum_{i=0}^{n} c_i \phi_i(x) \right\rangle + \int_a^b r(x)w(x)\,dx \\
&= \int_a^b r(x)w(x)\,dx
\end{aligned}$$

Generalized Rule Degree of Exactness $2n+1$

$$p(x) = \phi_{n+1}(x)q(x) + r(x), \qquad \int_a^b p(x)w(x)\,dx = \int_a^b r(x)w(x)\,dx.$$

Apply the $n+1$ point quadrature rule to p. (recall: $\deg(p) = 2n+1$)

$$\begin{aligned}
\int_a^b p(x)w(x)\,dx &\approx \sum_{j=0}^{n} w_j p(x_j) \\
&= \sum_{j=0}^{n} w_j \phi_{n+1}(x_j)q(x_j) + \sum_{j=0}^{n} w_j r(x_j) \\
&= \sum_{j=0}^{n} w_j \phi_{n+1}(x_j)q(x_j) + \int_a^b r(x)w(x)\,dx
\end{aligned}$$

If this sum is always 0, then

$$\sum_{j=0}^{n} w_j p(x_j) = \int_a^b r(x)w(x)\,dx = \int_a^b p(x)w(x)\,dx.$$

Generalized Rule Degree of Exactness $2n+1$

If we make

$$\sum_{j=0}^{n} w_j \phi_{n+1}(x_j) q(x_j) = 0$$

for any choice of nodes and weights, then the generalized $n+1$ point quadrature rule

$$\int_a^b f(x)w(x)\,dx \quad \approx \quad \sum_{j=0}^{n} f(x_j)w_j \qquad \text{where} \quad w_j = \int_a^b \ell_j(x)w(x)\,dx$$

has degree of exactness $2n+1$ because it is exact for all $p \in \mathcal{P}_{2n+1}$.

So, we choose the nodes $\{x_0, \ldots, x_n\}$ to be the roots of ϕ_{n+1}.

Gaussian Quadrature

Theorem 3

Let $\{\phi_0, \ldots, \phi_{n+1}\}$ *be a set of orthogonal polynomials on* $[a, b]$ *with respect to the weight function* $w(x)$. *Then* ϕ_k *has* k *distinct zeros in* $[a, b]$ *for each* $k = 0, 1, \ldots, n+1$.

Theorem 4 (Gaussian Quadrature)

Given n, *an interval* $[a, b]$, *and a weight function* $w(x)$, *choose the nodes* x_i *to be the* $n+1$ *roots of* ϕ_{n+1} *and the weights* w_i *to be* $w_i = \int_a^b \ell_i(x)w(x)\,dx$. *Then the quadrature rule*

$$\int_a^b f(x)w(x)\,dx \quad \approx \quad \sum_{j=0}^{n} w_j f(x_j)$$

is exact for all $f \in \mathcal{P}_{2n+1}$.

Observation: The nodes and weights do not depend on f!!

Generating Orthogonal Polynomials

How are the orthogonal polynomials $\{\phi_0, \ldots, \phi_{n+1}\}$ constructed?

Answer: Gram-Schmidt Algorithm, starting with $\phi_0 := 1$.

One can show the three-term recurrence:

$$\begin{aligned}
\phi_0 &= 1 \\
\phi_1 &= x - \frac{\langle x, 1\rangle}{\langle 1, 1\rangle} \\
\phi_k &= x\phi_{k-1} - \frac{\langle x\phi_{k-1}, \phi_{k-1}\rangle}{\langle \phi_{k-1}, \phi_{k-1}\rangle}\phi_{k-1} - \frac{\langle x\phi_{k-1}, \phi_{k-2}\rangle}{\langle \phi_{k-2}, \phi_{k-2}\rangle}\phi_{k-2}, \quad k \geq 2
\end{aligned}$$

Generating Orthogonal Polynomials

By shifting indices, then

$$\begin{aligned} \phi_{-1} &= 0 \\ \phi_0 &= 1 \\ \phi_{k+1} &= x\phi_k - \alpha_k \phi_k - \beta_k \phi_{k-1}, \qquad k \geq 0 \end{aligned}$$

where we define

$$\alpha_k = \frac{\langle x\phi_k, \phi_k \rangle}{\langle \phi_k, \phi_k \rangle} \quad \text{for } k \geq 0, \qquad \beta_k = \frac{\langle x\phi_k, \phi_{k-1} \rangle}{\langle \phi_{k-1}, \phi_{k-1} \rangle} \quad \text{for } k \geq 1.$$

Note that this recurrence generates monic polynomials.

Examples of Orthogonal Polynomials

For each weight function $w(x)$ there exists a system of orthogonal polynomials.

Weight	Interval	Orthogonal Polynomials
$w(x) = 1$	$[-1, 1]$	Legendre
$w(x) = \frac{1}{\sqrt{1-x^2}}$	$(-1, 1)$	Chebyshev
$w(x) = e^{-x}$	$(0, \infty)$	Laguerre
$w(x) = e^{-x^2}$	$(-\infty, \infty)$	Hermite

Example: Legendre Polynomials

When $w(x) = 1$ and $[a, b] = [-1, 1]$, we get the Legendre Polynomials.

One can show that

$$\alpha_k = \frac{\langle x\phi_k, \phi_k \rangle}{\langle \phi_k, \phi_k \rangle} = 0 \quad 0 \le k \le n, \qquad \beta_k = \frac{\langle x\phi_k, \phi_{k-1} \rangle}{\langle \phi_{k-1}, \phi_{k-1} \rangle} = \frac{k^2}{4k^2 - 1} \quad 1 \le k \le n$$

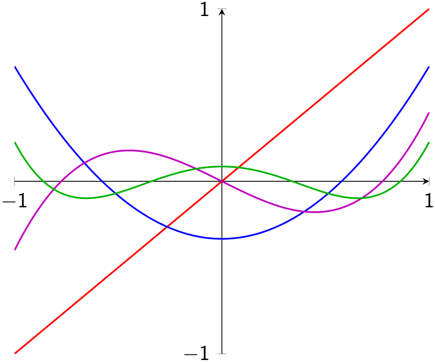
$$\phi_0(x) = 1$$

$$\phi_1(x) = x$$

$$\phi_2(x) = x^2 - \frac{1}{3}$$

$$\phi_3(x) = x^3 - \frac{3}{5}x$$

$$\phi_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}$$



Example: Chebyshev Polynomials

When $w(x) = \dfrac{1}{\sqrt{1-x^2}}$ and $[a, b] = (-1, 1)$, we get the Chebyshev Polynomials.

$$\alpha_k = 0 \quad 0 \le k \le n, \qquad \beta_k = \begin{cases} 1/2 & k = 1 \\ 1/4 & 2 \le k \le n \end{cases}, \qquad w_j = \frac{\pi}{n+1} \quad 0 \le j \le n$$

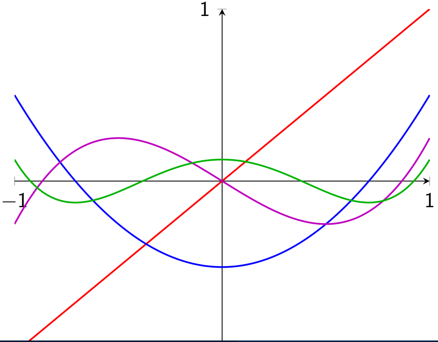
$$\phi_0(x) = 1$$

$$\phi_1(x) = x$$

$$\phi_2(x) = x^2 - \frac{1}{2}$$

$$\phi_3(x) = x^3 - \frac{3}{4}x$$

$$\phi_4(x) = x^4 - x^2 + \frac{1}{8}$$



Progress So Far

The orthogonal polynomials $\{\phi_0, \ldots, \phi_{n+1}\}$ can be generated cheaply via a three-term recurrence.

The nodes $\{x_0, \ldots, x_n\}$ can be chosen to be the roots of ϕ_{n+1}, and the weights $\{w_0, \ldots, w_n\}$ are found by $w_j = \int_a^b \ell_j(x) w(x)\, dx$.

Is there a way to more easily compute the nodes and weights?

The Tridiagonal Connection

From

$$\alpha_k = \frac{\langle x\phi_k, \phi_k \rangle}{\langle \phi_k, \phi_k \rangle} \quad \text{for } k \geq 0, \qquad \beta_k = \frac{\langle x\phi_k, \phi_{k-1} \rangle}{\langle \phi_{k-1}, \phi_{k-1} \rangle} \quad \text{for } k \geq 1$$

we define

$$\phi(x) = \begin{bmatrix} \phi_0(x) \\ \phi_1(x) \\ \vdots \\ \phi_n(x) \end{bmatrix}_{(n+1)\times 1} \qquad T = \begin{bmatrix} \alpha_0 & 1 & & & \\ \beta_1 & \alpha_1 & 1 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & \alpha_{n-1} & 1 \\ & & & \beta_n & \alpha_n \end{bmatrix}_{(n+1)\times(n+1)}.$$

Then

$$x\phi(x) = T\phi(x) + \phi_{n+1}(x) e_{n+1}.$$

The Tridiagonal Connection

$$x\phi(x) = T\phi(x) + \phi_{n+1}(x)e_{n+1}$$

Suppose $\phi_{n+1}(\lambda) = 0$. Then

$$\lambda\phi(\lambda) = T\phi(\lambda)$$

so $(\lambda, \phi(\lambda))$ is an eigenpair of T.

Quadrature Nodes $=$ Roots of $\phi_{n+1}(x)$ $=$ Evals. of T

The Tridiagonal Connection

Using a similarity transformation with

$$D = \operatorname{diag}\left(1\,,\ \sqrt{\beta_1}\,,\ \sqrt{\beta_1\beta_2}\,,\ \ldots\,,\ \sqrt{\beta_1\ldots\beta_n}\right)$$

then

$$D^{-1}TD := J = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \sqrt{\beta_2} & \ddots & \ddots & & \\ & & \ddots & \alpha_{n-1} & \sqrt{\beta_n} \\ & & & \sqrt{\beta_n} & \alpha_n \end{bmatrix}_{(n+1)\times(n+1)} .$$

If $(\lambda, \phi(\lambda))$ is an eigenpair of T, then $(\lambda, D^{-1}\phi(\lambda))$ is an eigenpair of J.

Calculating Weights

Eigenpairs of J are of the form $(\lambda, D^{-1}\phi(\lambda))$:

$$v := D^{-1}\phi(\lambda) = \begin{bmatrix} \phi_0(\lambda) \\ \phi_1(\lambda)/\sqrt{\beta_1} \\ \vdots \\ \phi_n(\lambda)/\sqrt{\beta_1 \dots \beta_n} \end{bmatrix}.$$

In 1969, Golub and Welsch proved that the weights w_i satisfy

$$w_i = \beta_0 \cdot \frac{v_{1i}^2}{\|v_i\|^2} \qquad 0 \leq i \leq n$$

where $\beta_0 = \langle 1, 1 \rangle = \int_a^b w(x)\, dx$.

Gaussian Quadrature

Given $f \in C[a, b]$, weight function $w(x)$, and integer n, form the matrix J

$$J = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \ddots & \ddots & \\ & & \ddots & \alpha_{n-1} & \sqrt{\beta_n} \\ & & & \sqrt{\beta_n} & \alpha_n \end{bmatrix}$$

with values defined by the three-term recurrence. Find eigenpairs (λ_i, v_i) of J. By choosing the nodes $x_i = \lambda_i$ and weights $w_i = \beta_0 \cdot \dfrac{v_{1i}^2}{\|v_i\|^2}$ then

$$\int_a^b f(x)w(x)\,dx = \sum_{j=0}^{n} w_j f(x_j)$$

for all $f \in \mathcal{P}_{2n+1}$.

Example: Gauss-Legendre Quadrature

Consider the interval $[-1,1]$ and $w(x)=1$. Recall that this generates the (monic) Legendre polynomials

$$\phi_0(x)=1, \qquad \phi_1(x)=x, \qquad \phi_2(x)=x^2-\frac{1}{3}, \qquad \ldots$$

by using

$$\alpha_k=0 \quad 0\le k\le n, \qquad \beta_k=\frac{k^2}{4k^2-1} \quad 1\le k\le n$$

Example: Gauss-Legendre Quadrature

For example, let $n = 4$. Then J is

$$J = \begin{bmatrix} 0 & 0.5774 & & & \\ 0.5774 & 0 & 0.5164 & & \\ & 0.5164 & 0 & 0.5071 & \\ & & 0.5071 & 0 & 0.5040 \\ & & & 0.5040 & 0 \end{bmatrix}.$$

Eigenvalues of J (nodes) and weights are

Nodes	-0.9062	-0.5385	0	0.5385	0.9062
Weights	0.2369	0.4786	0.5689	0.4786	0.2369

Example: Gauss-Legendre Quadrature

With $n = 4$, we can exactly integrate polynomials of degree $\leq 2n + 1 = 9$:

$$\int_{-1}^{1} x^9 + x^6 \, dx \quad = \quad \sum_{k=0}^{4} w_j f(x_j) \quad = \quad 0.2857$$

$$\int_{-1}^{1} x^{12} \, dx \qquad \text{Error:} \quad 0.008$$

$$\int_{-1}^{1} \sin(e^{x^2}) \, dx \qquad \text{Error:} \quad 9.9 \times 10^{-4}$$

Shifting to Other Intervals

Consider a rule on $[c, d]$, with nodes x_j, weights w_j, weight function $w(x)$.

We want to create a quadrature rule on $[a, b]$.

Define the affine transformation

$$\tau : [c, d] \to [a, b], \qquad \tau(x) = a + \frac{b-a}{d-c}(x-c)$$
$$\tau^{-1} : [a, b] \to [c, d], \qquad \tau^{-1}(y) = c + \frac{d-c}{b-a}(y-a)$$

Note that

$$\begin{aligned} \int_a^b f(x)w(x)\,dx &= \int_{\tau^{-1}(a)}^{\tau^{-1}(b)} f(\tau(x))w(\tau(x))\tau'(x)\,dx \\ &= \frac{b-a}{d-c}\int_c^d f(\tau(x))w(\tau(x))\,dx \end{aligned}$$

Shifting to Other Intervals

$$\int_a^b f(x)w(x)\,dx = \frac{b-a}{d-c}\int_c^d f(\tau(x))w(\tau(x))\,dx$$
$$= \frac{b-a}{d-c}\sum_{j=0}^{n} f(\tau(x_j))\,w_j$$

Then the nodes and weights for the $[a, b]$ quadrature rule are

$$\widehat{x}_j = \tau(x_j), \qquad \widehat{w}_j = \frac{b-a}{d-c}w_j$$

and the weight function is $\widehat{w}(x) = w(\tau(x))$. That is,

$$\int_a^b f(x)\widehat{w}(x)\,dx = \sum_{j=0}^{n} f(\widehat{x}_j)\widehat{w}_j.$$

Tridiagonal Eigenvalue Problem

Computing nodes and weights requires forming and computing eigenpairs of

$$J = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \ddots & \ddots & \\ & & \ddots & \alpha_{n-1} & \sqrt{\beta_n} \\ & & & \sqrt{\beta_n} & \alpha_n \end{bmatrix}$$

On the other hand, if we have an arbitrary symmetric tridiagonal matrix, what do quadrature weights of the matrix tell us?

Next Time

- In numerical linear algebra, one may wish to approximate extreme eigenpairs of a large symmetric matrix A using an iterative method.

- In short: Given $A \in \mathbb{R}^{n \times n}$ and $m \ll n$, then m extreme eigenpairs of A may be approximated by the eigenpairs of an $m \times m$ symmetric tridiagonal matrix T (called Ritz pairs).

- We are interested in how the Gaussian Weights of T may accelerate convergence of the Ritz pairs.

Questions?

Theorem 5

Let $\{\phi_0, \ldots, \phi_{n+1}\}$ be a set of orthogonal polynomials on $[a, b]$ with respect to the weight function $w(x)$. Then ϕ_k has k distinct zeros in $[a, b]$ for each $k = 0, 1, \ldots, n+1$.

Clearly the result holds for ϕ_0. Suppose by way of contradiction that ϕ_k changes sign on $[a, b]$ at j distinct roots $x_1, \ldots, x_j$ where $j < k$. Define

$$q(x) = (x - x_1)(x - x_2) \ldots (x - x_j) \in \mathcal{P}_j.$$

Note that q changes sign at $x_1, \ldots, x_j$ as well, so the product $q(x)\phi_k(x)$ does not change sign on $[a, b]$. Because $w(x) \geq 0$, then $q(x)\phi_k(x)w(x)$ does not change sign either on $[a, b]$. Because $q \in \mathcal{P}_j$ and $j < k$, then

$$\langle \phi_k, q \rangle = \int_a^b \phi_k(x)q(x)w(x)\, dx = 0$$

This suggests that a continuous nonzero function which never changes sign on $[a, b]$ has an integral that is zero, hence we have our contradiction. Therefore, ϕ_k has *at least* k distinct zeros in $[a, b]$, so it has precisely k.

Three-Term Recurrence

Suppose we have an orthogonal set $\{\phi_0, \dots, \phi_{k-1}\}$ and want ϕ_k. Note that $x\phi_{k-1}$ has degree k and is not in the span of $\{\phi_0, \dots, \phi_{k-1}\}$. Orthogonalize $x\phi_{k-1}$ against the previous $\{\phi_0, \dots, \phi_{k-1}\}$ to get

$$\phi_k(x) = x\phi_{k-1}(x) - \sum_{j=0}^{k-1} \frac{\langle x\phi_{k-1}(x), \phi_j(x)\rangle}{\langle \phi_j(x), \phi_j(x)\rangle}\phi_j(x). \tag{3}$$

Now, notice that we can move the x to the other slot in the inner product above because

$$\begin{aligned}\langle x\phi_{k-1}(x), \phi_j(x)\rangle &= \int_a^b x\phi_{k-1}(x)\phi_j(x)w(x)\,dx \\ &= \int_a^b \phi_{k-1}(x)x\phi_j(x)w(x)\,dx \\ &= \langle \phi_{k-1}(x), x\phi_j(x)\rangle\end{aligned}$$

In this inner product, if $j+1$ (the degree of the polynomial in the second slot) is less than $k-1$ (the degree of the polynomial in the first slot), then by orthogonality the inner product is zero. That is,

$$j+1 < k-1 \quad \Rightarrow \quad \langle \phi_{k-1}(x), x\phi_j(x) \rangle = 0.$$

Equivalently if $j < k-2$ then the inner product is zero. This means that we can move the starting index of the summation in (3) up to $k-2$:

$$\phi_k(x) = x\phi_{k-1}(x) - \sum_{j=k-2}^{k-1} \frac{\langle x\phi_{k-1}(x), \phi_j(x) \rangle}{\langle \phi_j(x), \phi_j(x) \rangle} \phi_j(x).$$