§ 10.3 Gauss Quadrature.

Idea: Find approximation for $\int_a^b f(x)dx$ by using both suitable x_i's and A_i's in the formula $\int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i)$. By "suitable" we mean finding the parameters s.t. this formula is exact for as high-degree polynomials as possible. (Named after Carl Friedrich Gauss, 1777 – 1855)

Consider $\boxed{n=0}$: $\int_a^b f(x)\,dx \approx A_0 f(x_0)$ (*)

Want (*) to be exact for constants (polynomials of degree 0) :

$$\int_a^b 1\,dx = \boxed{b-a = A_0}$$

Also let (*) be exact for polynomials of deg. 1:

$$\int_a^b x\,dx = \frac{b^2}{2} - \frac{a^2}{2} = \underbrace{A_0}_{= b-a} x_0 \Rightarrow \frac{b^2-a^2}{2} = (b-a)x_0$$

$\Rightarrow \boxed{x_0 = \frac{b+a}{2}}$. If A_0, x_0 are chosen in this way, then

$$\int_a^b x^2\,dx = \frac{b^3-a^3}{3} \neq \underbrace{(b-a)}_{A_0} \underbrace{\frac{(b+a)^2}{4}}_{x_0^2} \Rightarrow$$

(*) is not exact for polynomials of degree 2.

Thus, (*) is exact for polynomials of degree 0 and 1 (also called one-pt quadrature formula).

Now if $\boxed{n=1}$: $\int_a^b f(x)\,dx \approx A_0 f(x_0) + A_1 f(x_1)$ ②

We require:

$$\left.\begin{array}{l} \int_a^b 1\,dx = \boxed{b-a = A_0 + A_1} \\ \int_a^b x\,dx = \boxed{\frac{b^2-a^2}{2} = A_0 x_0 + A_1 x_1} \\ \int_a^b x^2\,dx = \boxed{\frac{b^3-a^3}{3} = A_0 x_0^2 + A_1 x_1^2} \\ \vdots \end{array}\right\}$$

system of non-linear equations!

Difficult to solve and to know how many equations are needed.

Gauss used a different approach.

§ 10.3.1 Orthogonal Polynomials.

Def. Polynomials p and q are orthogonal on $[a,b]$ if $\langle p,q\rangle = \int_a^b p(x)q(x)\,dx = 0$ and orthonormal if, in addition, $\langle p,p\rangle = \langle q,q\rangle = 1$.

Note: $\|p\| = \sqrt{\langle p,p\rangle} = \sqrt{\int_a^b p^2(x)\,dx}$

$\langle\cdot,\cdot\rangle$ is the dot product, $\|\cdot\|$ is the norm.

Gram-Schmidt algorithm for vectors:

see §7.6.2, also pp. 424-425

Given linearly independent vectors $v_1,\dots,v_n$, find orthonormal set $q_1,\dots,q_n$ by: $q_1 = \frac{v_1}{\|v_1\|}$, $q_j = \frac{\tilde{q}_j}{\|\tilde{q}_j\|}$, where

$$\tilde{q}_j = v_j - \sum_{i=1}^{j-1} \langle v_j, q_i\rangle q_i \quad , j \ge 1.$$

<u>Now:</u> given linearly independent set of polynomials $1, x, x^2, \dots,$ construct an orthonormal set $\underbrace{q_0}_{\deg 0}, \underbrace{q_1}_{\deg 1}, \underbrace{q_2}_{\deg 2}, \dots$ using Gram-Schmidt alg,

<u>namely:</u>

$$q_0 = \frac{1}{\sqrt{\int_a^b 1^2 dx}} = \frac{1}{\sqrt{b-a}}, \text{ Then:}$$

set $\tilde{q}_1(x) = xq_0 - \langle x, q_0 \rangle q_0 = \frac{x}{\sqrt{b-a}} - \left(\int_a^b \frac{x}{\sqrt{b-a}} dx\right) \frac{1}{\sqrt{b-a}}$

then $q_1(x) = \frac{\tilde{q}_1(x)}{\|\tilde{q}_1(x)\|}$

For $j \geq 1$, $\tilde{q}_j(x) = xq_{j-1}(x) - \sum_{i=0}^{j-1} \underbrace{\langle xq_{j-1}(x), q_i(x) \rangle}_{= \int_a^b xq_{j-1}(x) q_i(x) dx} q_i(x)$

& $q_j(x) = \frac{\tilde{q}_j(x)}{\underbrace{\|\tilde{q}_j(x)\|}_{= \left[\int_a^b (\tilde{q}_j(x))^2 dx\right]^{1/2}}}$

<u>Note:</u> since $q_{j-1} \perp$ all polynomials of deg. $j-2$ or less $\Rightarrow$ $\underset{i \leq j-3}{\langle xq_{j-1}(x), q_i(x) \rangle} = \langle q_{j-1}(x), \underbrace{xq_i(x)}_{\deg \leq j-2} \rangle$

$= 0 ! \Rightarrow$

$$\boxed{\begin{aligned} \tilde{q}_j(x) = xq_{j-1}(x) &- \langle xq_{j-1}(x), q_{j-2}(x) \rangle q_{j-2}(x) \\ &- \langle xq_{j-1}(x), q_{j-1}(x) \rangle q_{j-1}(x) \end{aligned}}$$

So, $\tilde{q}_j(x)$ depends on q_{j-1} & q_{j-2} ($\Rightarrow$ 3-term reccurence) $\Rightarrow$ q_j is obtained from q_{j-1} & q_{j-2}.

Once we get $q_0, q_1, \dots, q_{n+1}, \dots,$ let us discuss the following

Theorem (10.3.1)

If $x_0, x_1, \ldots, x_n$ are zeros of $q_{n+1}(x)$, the $(n+1)$st orthonormal polynomial on $[a,b]$, then the formula $\int_a^b f(x)\,dx \simeq \sum_{i=0}^{n} A_i f(x_i)$ where $A_i = \int_a^b \underbrace{\prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}}_{\varphi_i(x)} dx$, is exact for polynomials of degree $\underline{2n+1}$ or less.

Proof: Let f be a polyn. of deg $2n+1$ (or less).
If we divide f by q_{n+1}, then:

$$\underset{(2n+1)}{f} = \underset{(n+1)}{q_{n+1}}\ \underset{(n)}{p_n} + \underset{(n)}{r_n}$$

Since $q_{n+1}(x_i) \underset{i=0,\ldots,n}{=} 0 \Rightarrow f(x_i) = r_n(x_i) \rightarrow$

$$\int_a^b f(x)\,dx = \underbrace{\int_a^b q_{n+1}(x)\,p_n(x)\,dx}_{\overset{\shortparallel}{0} \text{ since } q_{n+1} \perp p_n} + \int_a^b r_n(x)\,dx = \int_a^b r_n(x)\,dx$$

If $A_i = \int_a^b \underbrace{\prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}}_{\deg} dx$ then $\int_a^b r_n(x)\,dx = \sum_{i=0}^{n} A_i \overbrace{r_n(x_i)}^{f(x_i)}$

$\left(\text{since } r_n(x) = \sum r_n(x_i) \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\right.$ Lagrange form $\Big)$

$\Rightarrow \int_a^b f(x)\,dx = \int_a^b r_n(x)\,dx = \sum_{i=0}^{n} A_i f(x_i) \Rightarrow$ formula exact for any polyn. of deg $2n+1$ (or less). $\square$

<u>Note:</u> When finding $x_0, \dots, x_n$, roots of q_{n+1}, we do not need to normalize $\tilde{q}_0, \dots, \tilde{q}_{n+1}$ since the roots of $\tilde{q}_i$ will be the roots of q_i. This is easier!

Consider the following formulas for $[a,b] = [-1,1]$, $n=1$ $\left(\Rightarrow \int_a^b f(x)\,dx = A_0 f(x_0) + A_1 f(x_1)\right.$ is exact for polynomials of deg $2n+1 = 3$ or less$\left.\right)$:

$$\tilde{q}_0(x) = \boxed{1},$$

$$\tilde{q}_1(x) = x - \frac{\langle x, \tilde{q}_0 \rangle}{\langle \tilde{q}_0, \tilde{q}_0 \rangle}\tilde{q}_0(x) = x - \frac{\overbrace{\int_{-1}^{1} x\,dx}^{=0}}{\int_{-1}^{1} 1\,dx} \cdot 1 = \boxed{x},$$

$$\tilde{q}_2(x) = x^2 - \frac{\langle x^2, \tilde{q}_0 \rangle}{\langle \tilde{q}_0, \tilde{q}_0 \rangle}\tilde{q}_0(x) - \frac{\langle x^2, \tilde{q}_1 \rangle}{\langle \tilde{q}_1, \tilde{q}_1 \rangle}\tilde{q}_1(x) =$$

$$= x^2 - \frac{\int_{-1}^{1} x^2\,dx}{\int_{-1}^{1} 1\,dx} \cdot 1 - \frac{\overbrace{\int_{-1}^{1} x^3\,dx}^{=0}}{\int_{-1}^{1} x^2\,dx} \cdot x$$

$$= x^2 - \frac{\frac{1}{3} + \frac{1}{3}}{2} - 0 = \boxed{x^2 - 1/3}.$$

Since $x_0 = -\frac{1}{\sqrt{3}}$, $x_1 = \frac{1}{\sqrt{3}}$ are roots of $\tilde{q}_2$, then

$$\int_a^b f(x)\,dx \approx A_0 \cdot f\left(-\frac{1}{\sqrt{3}}\right) + A_1 f\left(\frac{1}{\sqrt{3}}\right)$$

We can find A_0, A_1 using the method of undetermined coefficients:

$$\int_{-1}^{1} 1\,dx = 2 = A_0 + A_1$$
$$\int_{-1}^{1} x\,dx = 0 = A_0\left(-\frac{1}{\sqrt{3}}\right) + A_1\left(\frac{1}{\sqrt{3}}\right) \Rightarrow \begin{matrix} A_0 = 1 \\ A_1 = 1 \end{matrix}$$

(or use the formulas for A_0, A_1 from Thm. 10.3.1)

Thus, $\int_{-1}^{1} f(x)\,dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$ and it is exact for polynomials of deg 3 or less.

(Check: $\int_{-1}^{1} x^2\,dx = \frac{2}{3} = \left(-\frac{1}{\sqrt{3}}\right)^2 + \left(\frac{1}{\sqrt{3}}\right)^2$ ✓
$\int_{-1}^{1} x^3\,dx = 0 = \left(-\frac{1}{\sqrt{3}}\right)^3 + \left(\frac{1}{\sqrt{3}}\right)^3$ ✓, but $\int_{-1}^{1} x^4\,dx = \frac{2}{5} \neq$
$\left(-\frac{1}{\sqrt{3}}\right)^4 + \left(\frac{1}{\sqrt{3}}\right)^4 = 2/9$)

<u>Note:</u> $\forall n$, $\tilde{q}_n(x) = x^n - \frac{\langle x^n, \tilde{q}_0\rangle}{\langle \tilde{q}_0, \tilde{q}_0\rangle}\tilde{q}_0(x) - \dots - \frac{\langle x^n, \tilde{q}_{n-1}\rangle}{\langle \tilde{q}_{n-1}, \tilde{q}_{n-1}\rangle}\tilde{q}_{n-1}(x)$

($\tilde{q}_0, \tilde{q}_1, \dots$ found on $[-1,1]$)

are called the <u>Legendre polynomials.</u>

If $n=2$ then $\tilde{q}_3(x) = x^3 - \frac{\langle x^3, 1\rangle}{\langle 1, 1\rangle}(1) - \frac{\langle x^3, x\rangle}{\langle x, x\rangle}\cdot x$
$- \frac{\langle x^3, x^2 - 1/3\rangle}{\langle x^2 - \frac{1}{3}, x^2 - \frac{1}{3}\rangle}\left(x^2 - \frac{1}{3}\right) = x^3 - \frac{3}{5}x \Rightarrow$ roots are

$x_0 = -\sqrt{3/5}$, $x_1 = 0$, $x_2 = \sqrt{\frac{3}{5}}$. One can show that

$A_0 = A_2 = 0.5555556$, $A_1 = 0.8888889 \Rightarrow$

$\int_{-1}^{1} f(x)\,dx = A_0 f\left(-\sqrt{\frac{3}{5}}\right) + A_1 f(0) + A_2 f\left(\sqrt{\frac{3}{5}}\right)$ - exact for polynomials of degree $2\cdot 2+1 = 5$ or less.

If we require for the Legendre polynomials to satisfy $\tilde{q}_i(1) = 1$, then these are normalized (or standardized) polynomials:

$$p_0(x) = 1, \quad p_1(x) = x, \quad p_2(x) = \frac{1}{2}(3x^2 - 1),$$
$$p_3(x) = \frac{1}{2}(5x^3 - 3x), \ \ldots, \quad p_n(x) = \frac{1}{2^n \cdot n!} \frac{d^n}{dx^n}\left((x^2-1)^n\right)$$

- Weighted Orthogonal Polynomials.

Let $w(x) \geq 0$ on $[a,b]$. Then

$$\underbrace{\langle p, q \rangle_w = \int_a^b p(x)\, q(x)\, w(x)\, dx}_{\text{weighted dot product}}$$

If $\langle p, q \rangle_w = 0 \Rightarrow p \perp q$ w.r.t. $\underline{w}$

If one wants to approximate $\int_a^b f(x)\, w(x)\, dx$, then

$$\int_a^b f(x)\, w(x)\, dx \simeq \sum_{i=0}^{n} A_i f(x_i) \quad \text{where}$$

$$A_i = \int_a^b \varphi(x)\, w(x)\, dx, \quad \varphi_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

and $x_0, \ldots, x_n$ are zeros of $(n+1)$ st w-orthogonal polynomial on $[a,b]$ (Thm. 10.3.2)

(exact for polyn. of deg $2n+1$ or less)

so-called $\underline{\text{weighted Gauss quadrature formula}}$

<u>Example</u>: $[a,b] = [-1,1]$, $w(x) = (1-x^2)^{-1/2}$, $n = 1$

$$\int_{-1}^{1} f(x)\, w(x)\, dx \simeq A_0 f(x_0) + A_1 f(x_1)$$

$\rightarrow$ must be exact for polyn. of deg 3 or less

Need: $\tilde{q}_0, \tilde{q}_1, \tilde{q}_2$, w-orthogonal on $[-1,1]$. (8)

So, if $\tilde{q}_0 = 1$, then $\tilde{q}_1 = x - \frac{\langle x,1\rangle_w}{\langle 1,1\rangle_w} \cdot 1$

$$= x - \frac{\int_{-1}^{1} x/\sqrt{1-x^2}\,dx}{\int_{-1}^{1} 1/\sqrt{1-x^2}\,dx} = x,$$

$$\tilde{q}_2 = x^2 - \frac{\langle x^2,1\rangle_w}{\langle 1,1\rangle_w} \cdot 1 - \frac{\langle x^2,x\rangle_w}{\langle x,x\rangle_w} \cdot x = x^2 - \frac{1}{2} \Rightarrow$$

$$x_0 = -\frac{1}{\sqrt{2}},\ x_1 = \frac{1}{\sqrt{2}} \Rightarrow$$

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\,dx \approx A_0 f\left(-\tfrac{1}{\sqrt{2}}\right) + A_1 f\left(\tfrac{1}{\sqrt{2}}\right)$$

By the method of undetermined coeff's,

$A_0 = A_1 = \pi/2$ (Try it!)

Thus, $$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\,dx \approx \frac{\pi}{2} f\left(-\tfrac{1}{\sqrt{2}}\right) + \frac{\pi}{2} f\left(\tfrac{1}{\sqrt{2}}\right) \qquad (**)$$

(Check if $(**)$ exact for $f(x) = x^2$ and x^3, but not for x^4.)

<u>Note</u>: these $\tilde{q}_0, \tilde{q}_1, \tilde{q}_2, \ldots$, w-orthogonal on $[-1,1]$, are called Chebyshev (or Tschebyscheff) polynomials. Standardization $\tilde{q}_i(1) = 1$ gives

$$\tilde{q}_0 \to T_0(x) = 1$$
$$\tilde{q}_1 \to T_1(x) = x$$
$$\tilde{q}_2 \to T_2(x) = 2x^2 - 1$$
$$\ldots$$

(In general, $T_j(x) = \cos(j \arccos x)$, $j = 0, 1, 2, \ldots$)