(57) 3/1/2017>

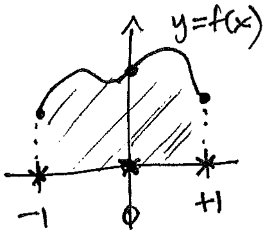
§4.6 Numerical integration methods

– what to do when no antiderivatives around (most of the time!)

Simpson's rule came from trying to evaluate f at 3 regularly spaced points and take a linear combination matching $\int_{-1}^{+1} f(x)\,dx$

i.e. want c_{-1}, c_0, c_{+1} so that

$$\int_{-1}^{+1} f(x)\,dx \approx c_{-1}f(-1) + c_0 f(0) + c_{+1}f(+1)$$



Since 3 unknowns, can make this exact for $f(x)$ a quadratic polynomial, i.e. a linear combination of $1, x, x^2$:

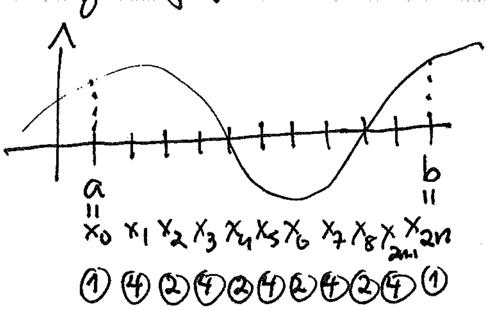
$$\left.\begin{aligned}
\int_{-1}^{1} 1\cdot dx = 2 &= c_{-1} + c_0 + c_{+1} \\
\int_{-1}^{1} x\,dx = 0 &= c_{-1}(-1) + c_0(0) + c_{+1}(+1) \\
\int_{-1}^{1} x^2\,dx = \left[\frac{x^3}{3}\right]_{-1}^{1} = \frac{2}{3} &= c_{-1}(-1)^2 + c_0(0)^2 + c_{+1}(+1)^2
\end{aligned}\right\} \xRightarrow{\text{solve}} \begin{aligned} c_{-1} &= 1 \\ c_0 &= 4 \\ c_{+1} &= 1 \end{aligned}$$

BONUS:

$$\int_{-1}^{1} x^3\,dx = 0 = 1\cdot(-1)^3 + 4(0)^3 + 1(+1)^3$$, so it's also exact for cubics on $[-1,+1]$.

DEF'N 4.6.1
THM 4.6.2: If we define Simpson's approximation for $\int_a^b f(x)\,dx$ with $2n+1$ equally spaced points as

$$S^n_{[a,b]}(f) := \frac{b-a}{6n}\Big[1\cdot f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 4f(x_{2n-1}) + 1\cdot f(x_{2n})\Big]$$



then (i) $\int_a^b f(x)\,dx = S^n_{[a,b]}(f)$ for cubic polynomials f

For $f \in C^4[a,b]$,

(ii) $$S^n_{[a,b]}(f) - \int_a^b f(x)\,dx = \frac{(b-a)^5}{4\cdot 6!}\,\frac{f^{(4)}(c)}{n^4}$$ for some $c \in (a,b)$

shrinks rapidly as n grows

proof: We'll only check (i), but EXER. 4.6.6 leads one through a proof of (ii).

Note $\displaystyle\int_a^b f(x)\,dx = \int_{\substack{x_0\\ \| \\ a}}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{2n-2}}^{\substack{b\\ \| \\ x_{2n}}} f(x)\,dx$

and $S^n_{[a,b],f} = S^1_{[x_0,x_2],f} + S^1_{[x_2,x_4],f} + \cdots + S^1_{[x_{2n-2},x_{2n}],f}$

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so enough to check $n=1$ case, i.e.

that $\displaystyle\int_a^b f(x)\,dx = S^1_{[a,b],f} = \frac{b-a}{6}\left[1\cdot f(a) + 4 f\left(\tfrac{a+b}{2}\right) + 1\cdot f(b)\right]$ for cubic f

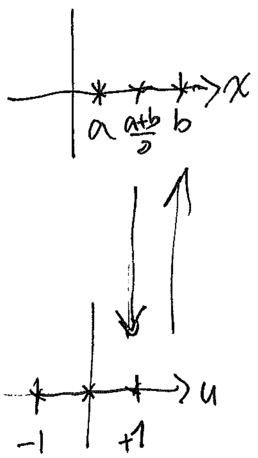
But $\displaystyle\int_{x=a}^{x=b} f(x)\,dx \underset{\text{substitute}}{=} \frac{b-a}{2}\int_{u=-1}^{u=+1} \underbrace{f\left(\frac{(b-a)u+(a+b)}{2}\right)}_{\substack{\text{call this } g(u),\\ \text{a cubic polynomial in } u}} du \underset{\text{already checked!}}{=} \frac{b-a}{2}\cdot\frac{(+1)-(-1)}{6}\left[g(-1)+4g(0)+g(+1)\right]$

$\displaystyle = \frac{b-a}{6}\left[f(a)+4f\left(\tfrac{a+b}{2}\right)+f(b)\right]$ ∎

substitute

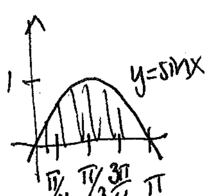
$u = \dfrac{2x-(a+b)}{b-a}$, $x = \dfrac{(b-a)u+(a+b)}{2}$

$du = \dfrac{2}{b-a}dx$, $dx = \dfrac{b-a}{2}du$



EXAMPLE: Simpson with $n=1$ already does OK approximating $\displaystyle\int_0^{\pi} \sin(x)\,dx \quad \left(= \left[-\cos x\right]_0^{\pi} = 1-(-1) = 2\right)$

since $S^1_{[0,\pi],\sin(x)} = \dfrac{\pi-0}{6}\left[\cancel{\sin(0)}^{\,0} + 4\underbrace{\sin\left(\tfrac{\pi}{2}\right)}_{=1} + \cancel{\sin(\pi)}^{\,0}\right] = \dfrac{4\pi}{6} = \dfrac{2}{3}\pi \approx 2.0944$,



but with $n=2$ it does much better:

$S^2_{[0,\pi],\sin(x)} = \dfrac{\pi-0}{6\cdot 2}\left[\cancel{\sin(0)}^{\,0} + 4\underbrace{\sin\left(\tfrac{\pi}{4}\right)}_{\frac{\sqrt{2}}{2}} + 2\underbrace{\sin\left(\tfrac{\pi}{2}\right)}_{=1} + 4\underbrace{\sin\left(\tfrac{3\pi}{4}\right)}_{\frac{\sqrt{2}}{2}} + \cancel{\sin(\pi)}^{\,0}\right]$

$= \dfrac{\pi}{12}\left[4\sqrt{2}+2\right] \approx 2.00456$

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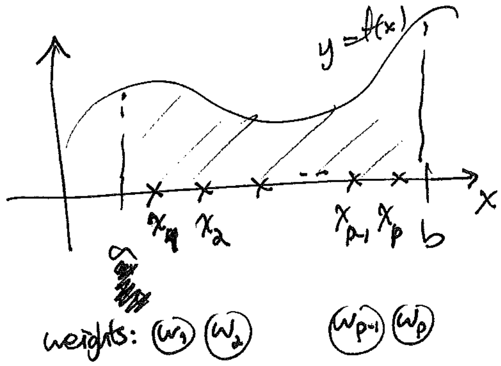
Gaussian quadrature

What if we <u>don't</u> <u>fix</u> the evaluation points on $[a,b]$ for $f(x_i)$?:

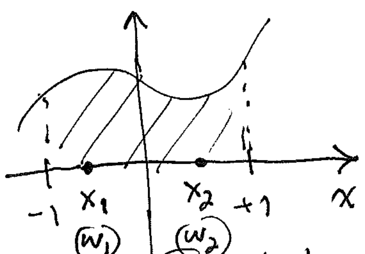


$$\int_a^b f(x)\,dx \approx w_1 f(x_1) + \dots + w_p f(x_p)$$

If we want it <u>exact</u> for polynomials $f(x) = a_0 + a_1 x + \dots + a_d x^d$ of degree d, then we could try to solve for the <u>$2p$ unknowns</u> $w_1, \dots, w_p, x_1, \dots, x_p$ using <u>$d+1$ equations</u>

$$\int_a^b x^i\,dx = w_1 x_1^i + \dots + w_p x_p^i \quad \text{for } i = 0, 1, \dots, d$$

whenever $2p = d+1$.



<u>Simplest case:</u> $p = 2$, $d = 3$, and try $[a,b] = [-1,+1]$ i.e. $\int_{-1}^{+1} x^i\,dx = w_1 x_1^i + w_2 x_2^i$, $i = 0, 1, 2, 3$

$$\left.\begin{array}{ll} i=0: & 2 = w_1 + w_2 \\ i=1: & 0 = w_1 x_1 + w_2 x_2 \\ i=2: & 2/3 = w_1 x_1^2 + w_2 x_2^2 \\ i=3: & 0 = w_1 x_1^3 + w_2 x_2^3 \end{array}\right\}$$

<u>nonlinear</u>, but not <u>too bad</u> (particularly if you guess $x_1 = -x_2$, $w_1 = w_2$)

$$\Longrightarrow w_1 = w_2 = 1, \quad x_1 = -x_2 = \frac{1}{\sqrt{3}}$$

i.e.

$$\boxed{\int_{-1}^{1} f(x)\,dx \underset{\left(\text{for } p=2,\ d=3\right)}{\overset{\text{Gauss quadrature}}{\approx}} 1\cdot f\left(\frac{-1}{\sqrt{3}}\right) + 1\cdot f\left(\frac{+1}{\sqrt{3}}\right)}$$

<u>EXAMPLE:</u> (4.6.4 in book)

$$\int_{-1}^{1} e^x\,dx = e^1 - e^{-1} \approx 2.3504$$

$$\overset{\text{Simpson}}{\underset{n=1}{\approx}} \frac{+1-(-1)}{6}\left(1\cdot e^{-1} + 4e^0 + 1\cdot e^{+1}\right) = \frac{1}{3}\left(e^{-1} + 4 + e^1\right) \approx 2.36205 \quad \text{not bad}$$

$$\overset{\text{Gauss quad.}}{\approx} 1\cdot e^{\frac{-1}{\sqrt{3}}} + 1\cdot e^{\frac{+1}{\sqrt{3}}} \approx 2.3427 \quad \text{better!}$$

There are also Gauss quadrature rules for a given prob. <u>density</u> $\mu(x)$, i.e. made to approximate $\int_a^b f(x)\mu(x)\,dx \approx \sum_{i=1}^{p} w_i f(x_i)$, <u>exact</u> for polynomials f with $\deg(f) \le d$.