$$\left(\sum_{j}^{N-1} \frac{\phi_k(x_j)\phi_\ell(x_j)}{\sigma_j^2} \right) = \sum_{j}^{N-1} A_{jk} A_{j\ell} = (A^T A)_{k\ell}$$
$$= U_{k\ell}$$

$$\sigma_{c_i}^2 = \sum_{k}^{n-1} \sum_{\ell}^{n-1} V_{ik} V_{i\ell} U_{k\ell}$$
$$= \sum_{\ell}^{n-1} V_{i\ell} \underbrace{\sum_{k}^{n-1} V_{ik} U_{k\ell}}_{} = \sum_{\ell}^{n-1} V_{i\ell}\, \delta_{i\ell} = V_{ii}$$

V is U^{-1} so product is $\mathbb{I}$

$$\sigma_{c_i}^2 = V_{ii} = [(A^T A)^{-1}]_{ii}$$

diagonal elements of V are the squared uncertainty of coeffs

V is <u>covariance</u> matrix

depends on model ϕ_k and uncertainties σ_j

[See newnormal.py]

Let's sketch more general solution

N data points (x_j, y_j, σ_j) $\quad$ n params c_k

define $\rho_j = \frac{p(x_j)}{\sigma_j}$ $\quad b_j = y_j/\sigma_j$

$$\chi^2(\vec{c}) = (\vec{b} - \vec{\rho})^T(\vec{b} - \vec{\rho}) = \sum^{N-1} (b_j - \rho_j)^2$$ same as before

recall we wrote solution for $\nabla\phi(\vec{x}) = 0$

$$J_{\nabla\phi}(\vec{x}^{(k-1)})(\vec{x}^{(k)} - \vec{x}^{(k-1)}) = -\nabla\phi(\vec{x}^{(k-1)})$$

$$\Rightarrow J_{\nabla\chi^2}(\vec{c}^{(k-1)})[\vec{c}^{(k)} - \vec{c}^{(k-1)}] = -\nabla\chi^2(\vec{c}^{(k-1)})$$

$$J_{f(x)} = \left\{ \frac{\partial f_j}{\partial x_k} \right\}$$

We introduce $K_\rho(\vec{c}) = \left\{ \frac{\partial \rho_j}{\partial c_k} \right\}$ $\quad N \times n$

$$\begin{matrix} \frac{\partial \rho_0}{\partial c_0} & \cdots & \frac{\partial \rho_0}{\partial c_{n-1}} \\ \vdots & & \vdots \\ \frac{\partial \rho_{N-1}}{\partial c_0} & \cdots & \frac{\partial \rho_{N-1}}{\partial c_{n-1}} \end{matrix}$$

and recall

$$\nabla\chi^2(\vec{c}) = \left[\frac{\partial\chi^2}{\partial c_0}, \ldots, \frac{\partial\chi^2}{\partial c_{n-1}} \right]^T$$

$$\partial\chi^2/\partial c_0 = -2\sum_j (b_j - \rho_j)\, \partial\rho_j/\partial c_0$$

$$\nabla\chi^2 = -2K_\rho^T[\vec{b} - \vec{\rho}]$$

$L_{\rho_j}(\vec{c}) = \left\{ \frac{\partial \rho_j}{\partial c_k \partial c_\ell} \right\}$ $n \times n$, one for each N

$J_{\nabla \chi^2}(\vec{c}) = \frac{\partial (\nabla \chi^2)_\ell}{\partial c_k}$

lots of algebra $J_{\nabla \chi^2}(\vec{c}) = 2 K_\rho^T K_\rho - 2 \sum^{N-1} (b_j - \rho_j) L_{\rho_j}$

as we iterate $b_j - \rho_j$ should get close to zero

$J_{\nabla \chi^2}(\vec{c}^{(k-1)}) \approx 2 K_\rho^T K_\rho$

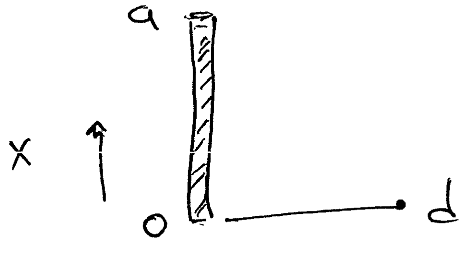
$$\Rightarrow \quad \underbrace{K_\rho^T K_\rho}_{n \times n} \underbrace{\left[\vec{c}^{(k)} - \vec{c}^{(k-1)} \right]}_{n \times 1} = \underbrace{K_\rho^T \left[\vec{b} - \vec{\rho} \right]}_{n \times 1}$$

$A\vec{x} = \vec{b}$ use gaussian elimination to find each iteration $\vec{c}^{(k)}$

Integrals

They come up in a lot of physics problems!

Find the potential a distance d from the end of a uniformly charged rod of length a.



Break into chunks of charge

$$dq = \lambda\, dx$$

$$V(r) = k \int dq/r = k\lambda \int_0^a \frac{dx}{\sqrt{d^2+x^2}}$$

$k = 1/4\pi\epsilon_0$

$$V(r) = k\lambda \int_0^a \frac{dx}{d\sqrt{1+(x/d)^2}} \quad \text{let } y = x/d$$

$$V(r) = \frac{k\lambda}{d}\int_0^{a/d} \frac{d\, dy}{\sqrt{y^2+1}} = k\lambda \ln\left(a/d + \sqrt{(a/d)^2+1}\right)$$

Maxwell Boltzmann ideal gas velocity (1D)

$$P(v_x) = \sqrt{\frac{M}{2\pi kT}}\, e^{-Mv_x^2/2kT}$$

integrate dv_x over some range to get probability

$$\int_{-a}^{a} P(v_x)\, dv_x \Rightarrow \text{not analytic, error function}$$

We will solve $\int_a^b f(x)\,dx$ by approximating

as $\sum_i^{n-1} c_i f(x_i)$ $\qquad x_i$ = nodal abscissas

$c_i \equiv$ weights

closed methods $\Rightarrow$ a, b are abscissas

open methods $\Rightarrow$ a, b are not abscissas

Newton-Cotes Methods

integral = sum of areas of rectangles, trapezoids, etc

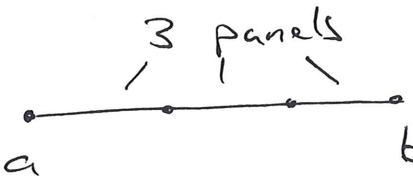
consider n equally spaced points x_i $\quad i = 0, 1, \ldots n-1$

with $x_i = a + ih$ and $h = \dfrac{b-a}{n-1}$

$(x_0 = a, \; x_{n-1} = b)$

we can introduce $N \equiv$ # of panels $= n-1$

$n = 4$

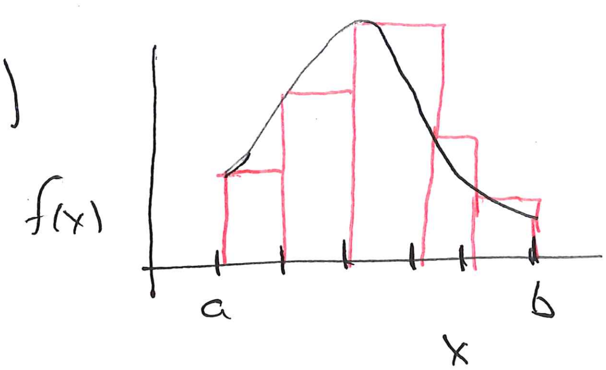


$N = 3$

- rectangle rule

$N = 1$ $\quad \displaystyle\int_{x_i}^{x_{i+1}} f(x)\,dx \approx h\, f(x_i)$

we are evaluating on LHS



total (composite) integral

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-2} \int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$\approx h\, f(x_0) + h\, f(x_1) + \ldots h\, f(x_{n-2})$$

(can't do evaluation at x_{n-1})

<u>Error</u> Taylor expand $f(x)$ around x_i

$$f(x) = f(x_i) + (x - x_i) f'(x_i) + \dots$$

1st order $\quad f(x) = f(x_i) + (x - x_i) f'(\xi_i)$

ξ is a point between x and x_i

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \int_{x_i}^{x_{i+1}} dx\,[f(x_i) + (x - x_i) f'(\xi_i)]$$

let $u = \dfrac{x - x_i}{h}$ $\qquad x = x_i \Rightarrow u = 0 \qquad h\,du = dx$

$\qquad\qquad\qquad\qquad x = x_{i+1} \Rightarrow u = 1$

$$= \int_0^1 h\,du\,[f(x_i) + uhf'(\xi_i)]$$

$$= h f(x_i) + \tfrac{1}{2} h^2 f'(\xi_i)$$

absolute error in one panel $\left[\text{since } \int_{x_i}^{x_{i+1}} f(x)\,dx \approx h f(x_i)\right]$

is $\quad \varepsilon_i = \frac{1}{2} h^2 f'(\xi_i)$

total error $\quad \varepsilon = \sum \varepsilon_i = \frac{1}{2} h^2 \sum_0^{n-2} f'(\xi_i)$

calculus tells us there is a ξ in $[a, b]$ such that

$$f'(\xi) = \frac{\sum_0^{n-2} f'(\xi_i)}{n-1}$$

$$\Rightarrow \varepsilon = \frac{n-1}{2} h^2 f'(\xi) = \boxed{\frac{b-a}{2} h f'(\xi)}$$

Midpoint rule

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx h\, f(x_i + h/2)$$

expand $f(x)$ about $x_i + h/2 \equiv \Delta_i$

$$f(x) \approx f(\Delta_i) + (x-\Delta_i) f'(\Delta_i) + \frac{1}{2}(x-\Delta_i)^2 f''(\xi_i)$$

let $u = \dfrac{x-\Delta_i}{h/2}$ follow same steps (HW problem)

$$\varepsilon_i = \frac{1}{24} h^3 f''(\xi_i) \Rightarrow \varepsilon_{TOTAL} = \frac{b-a}{24} h^2 f''(\xi)$$

Trapezoid rule

Use straight line instead of constant for function

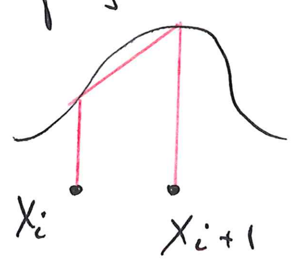
1 panel w/ 2 abscissas determine line

We will use Lagrange interpolation

General: q data points $x_{i+j}, f(x_{i+j})$ $j = 0, 1, .. q-1$

and we need interpolating polynomial

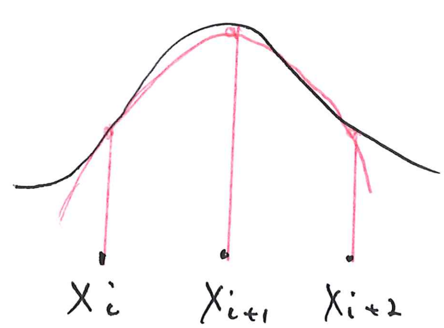
$q = 2 \Rightarrow$ line



$q = 3 \Rightarrow$ quadratic

In elementary interval

$\int_{x_i}^{x_{i+q-1}} f(x)\,dx$ needs to be approximated



approx $\int_{x_i}^{x_{i+q-1}} f(x)\,dx$ w/ $p(x) = \sum_{j=0}^{q-1} f(x_{i+j}) L_{i+j}(x)$

recall $L_k(x) = \dfrac{\prod_{j=0,\ j\neq k}^{n-1} (x-x_j)}{\prod_{\text{same}} (x_k - x_j)}$ $\Rightarrow$ $L_{i+j}(x) = \dfrac{\prod_{k=0,\ k\neq j}^{q-1} (x - x_{i+k})}{\prod (x_{i+j} - x_{i+k})}$

$k = 0, 1, \ldots n-1$ $\qquad$ $j = 0, 1, \ldots q-1$

$q = 3$ $\quad L_i(x), L_{i+1}(x), L_{i+2}(x)$ each is quadratic

to interpolate over x_i, x_{i+1}, x_{i+2}

$$\int_{x_i}^{x_{i+q-1}} f(x)\,dx \approx \int_{x_i}^{x_{i+q-1}} p(x)\,dx = \sum_{j=0}^{q-1} f(x_{i+j}) \int_{x_i}^{x_{i+q-1}} L_{i+j}(x)\,dx$$

$$= \sum_{j=0}^{q-1} \omega_{i+j} f(x_{i+j})$$

with $\omega_{i+j} \equiv \int_{x_i}^{x_{i+q-1}} L_{i+j}(x)\,dx$ $\Rightarrow$ do not depend on $f(x)$

We can find weights for a given q <u>once</u>

Let $q = 2$ (trapezoid)

$$L_i(x) = \frac{x - x_{i+1}}{\underbrace{x_i - x_{i+1}}_{-h}} \qquad L_{i+1}(x) = \frac{x - x_i}{\underbrace{x_{i+1} - x_i}_{h}}$$

$j = 0$ $\quad k = 1$ $\qquad\qquad$ $j = 1$ $\quad k = 0$

$$\omega_i = \int_{x_i}^{x_{i+1}} L_i(x)\,dx = -\frac{1}{h}\int_{x_i}^{x_i+h} (x - x_{i+1})\,dx$$

$$= -\frac{1}{h}\left[\tfrac{1}{2}x^2 - x\,x_{i+1}\right]_{x_i}^{x_i+h}$$

$$= -\frac{1}{h}\left[\frac{1}{2}(x_i+h)^2 - \frac{1}{2}x_i^2 - x_{i+1}h\right]$$

$$= -\frac{1}{h}\left[x_i h + \frac{1}{2}h^2 - x_{i+1}h\right] = -\frac{1}{h}\left[h(-h) + \tfrac{1}{2}h^2\right]$$

$$= h/2$$

$$\omega_{i+1} = \int_{x_i}^{x_{i+1}} L_{i+1}(x)\,dx = \frac{1}{h}\int_{x_i}^{x_{i+1}} (x - x_i)\,dx = h/2$$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \sum_{j=0}^{q-1} \omega_{i+j} f(x_{i+j}) = \frac{h}{2}\left[f(x_i) + f(x_{i+1})\right]$$

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-2} \int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$\approx \frac{h}{2}\left[f(x_0) + f(x_1) + f(x_1) + f(x_2) + f(x_2) + f(x_3) + \dots + f(x_{n-2}) + f(x_{n-1})\right]$$

$$\approx \frac{h}{2} f(x_0) + h f(x_1) + h f(x_2) + \dots h f(x_{n-2}) + \frac{h}{2} f(x_{n-1})$$

cummalitive set of weights $\left[\int_a^b f(x)\,dx \approx \sum_{i=0}^{n-1} c_i f(x_i)\right]$

$$c_i = h\left\{\frac{1}{2}, 1, 1, \dots 1, \tfrac{1}{2}\right\}$$

Simpson's rule : $q = 3$, quadratic

(2 panels)

$$L_i(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} \qquad L_{i+1}(x) = \frac{(x - x_i)(x - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}$$

$$L_{i+2}(x) = \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}$$

define $u = \frac{1}{h}(x - x_{i+1})$

$$w_i = \int_{x_i}^{x_{i+2}} L_i(x)\,dx = \frac{h}{2}\int_{-1}^{1} du\,(u-1)u = h/3$$

$$w_{i+1} = -h\int_{-1}^{1} du\,(u+1)(u-1) = 4h/3$$

$$w_{i+2} = \frac{h}{2}\int_{-1}^{1} du\,(u+1)u = h/3$$

$$\int_{x_i}^{x_{i+2}} f(x)\,dx \approx \frac{h}{3}\left[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})\right]$$

$$\int_a^b f(x)\,dx = \sum_{i=0,2,4}^{n-3} \int_{x_i}^{x_{i+2}} f(x)\,dx$$

$$\begin{array}{ccccccccc} x_0 & x_1 & x_2 & x_3 & x_4 & \cdots \\ 1/3 & 4/3 & 1/3 & & & \\ & & 1/3 & 4/3 & 1/3 & \\ & & & & 1/3 & 4/3 & 1/3 \end{array}$$

$$c_i = \frac{h}{3}\{1, 4, 2, 4, 2, 4, 2, \ldots, 2, 4, 1\}$$

[See code]