## Overview

- Weighted quadrature - method of moments
- Optimal sampling - Gauss quadrature
- Common Gauss quadrature methods:
  - Gauss-Legendre $\int_{-1}^{1} f(t)\,\mathrm{d}t$
  - Gauss-Chebyshev $\int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}\,\mathrm{d}t$
  - Gauss-Laguerre $\int_{0}^{\infty} e^{-t} f(t)\,\mathrm{d}t$
  - Gauss-Legendre $\int_{-\infty}^{\infty} e^{-t^2} f(t)\,\mathrm{d}t$

- $f: \mathbb{R} \rightarrow \mathbb{R}$ known through data set ($f$ sample) $\mathcal{D} = \{(x_i, f_i), i = 0, 1, \ldots, n\}$

$$\int_a^b f(t)\,\mathrm{d}t \cong \sum_{i=0}^{n} \left( \int_a^b \ell_i(t)\,\mathrm{d}t \right) f_i = \sum_{i=0}^{n} w_i\, f_i$$

- Set a simple, predefined integration domain, e.g., $[0, 1]$, $x_i = i\,h$, $h = 1/n$
- Monomial basis set: $\mathcal{M} = \{1, t, t^2, \ldots\}$ conditions

$$\begin{aligned} f(t) = 1:&\quad \int_0^1 1\,\mathrm{d}t &=& \ 1 &=& \sum_{i=0}^{n} w_i \\ f(t) = t:&\quad \int_0^1 t\,\mathrm{d}t &=& \ \frac{1}{2} &=& h \sum_{i=0}^{n} w_i\, i \\ f(t) = t^2:&\quad \int_0^1 t^2\,\mathrm{d}t &=& \ \frac{1}{3} &=& h \sum_{i=0}^{n} w_i\, i^2 \\ &\ldots. \end{aligned}$$

- Solve above system to find weights $w_i$, obtain formula with error $e \propto \| f^{(n)} \|_\infty$
- What if $f^{(n)}$ is not defined (infinite) at some points in the integration domain?

- Consider integrals of form

$$I_{\mathrm{ab}}(f) = \int_a^b \omega(t)\, f(t)\mathrm{d}t$$

- Typically:
  - $f$ is smooth, e.g., $f \in C^\infty[a,b]$ (all derivatives exist, are finite)
  - $w$ captures some *singular* behavior of the integral
- Examples:
  - Chebyshev weight

$$T(f) = \int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}\,\mathrm{d}t$$

  - Laguerre weight

$$L(f) = \int_0^\infty e^{-t} f(t)\,\mathrm{d}t$$

  - Hermite weight

$$H(f) = \int_{-\infty}^{\infty} e^{-t^2} f(t)\,\mathrm{d}t$$

- As in the $\omega(t)=1$ case, choose $f$ evaluation points, $x_i=a+ih$,$h=(b-a)n$
- Choose a basis set, e.g., monomials $\mathcal{M}=\{1,t,t^2,\ldots\}$ and impose exact result when using exact, analytical weight function $\omega(t)$
- Example for Chebyshev, $\omega(t)=(1-t^2)^{-1/2}$, $x_i=ih-1$, $h=2/n$, $i=0,\ldots,n$

$$f(t)=1:\quad \int_{-1}^{1}\omega(t)1\,\mathrm{d}t = \int_{-1}^{1}\frac{1}{\sqrt{1-t^2}}\,\mathrm{d}t = \pi = \sum_{i=0}^{n} w_i$$

$$f(t)=t:\quad \int_{-1}^{1}\omega(t)\,t\,\mathrm{d}t = \int_{-1}^{1}\frac{t}{\sqrt{1-t^2}}\,\mathrm{d}t = 0 = \sum_{i=0}^{n} w_i\,(ih-1)$$

$$f(t)=t^2:\quad \int_{-1}^{1}\omega(t)t^2\,\mathrm{d}t = \int_{-1}^{1}\frac{t^2}{\sqrt{1-t^2}}\,\mathrm{d}t = \frac{\pi}{2} = \sum_{i=0}^{n} w_i(ih-1)^2$$

$$\ldots.$$

- Up to now the sampling points $x_i$ were *arbitrarily* chosen

$$I_{\mathrm{ab}}(f) = \int_a^b f(t)\,\mathrm{d}t \cong Q_{\mathrm{ab}}(f) = \sum_{i=0}^{n} w_i\, f(x_i)$$

- One could obtain more accurate method by optimal choice of $x_i$, more of the moment equations could be satisfied, $2(n+1)$ instead of only $n+1$
- Difficult to do within method of moments since a non-linear system results

$$\begin{aligned}
f(t)=1:&\quad \int_0^1 1\,\mathrm{d}t &= 1 &= \sum_{i=0}^{n} w_i \\
f(t)=t:&\quad \int_0^1 t\,\mathrm{d}t &= \frac{1}{2} &= \sum_{i=0}^{n} w_i\, x_i \\
f(t)=t^2:&\quad \int_0^1 t^2\,\mathrm{d}t &= \frac{1}{3} &= \sum_{i=0}^{n} w_i\, x_i^2 \\
\ldots.
\end{aligned}$$

- Solving the nonlinear system can be avoided by use of orthogonal polynomials
- Consider

$$I_{\mathrm{ab}}(f) = \int_a^b \omega(t) f(t)\,\mathrm{d}t \cong Q_{\mathrm{ab}}(f) = \sum_{i=0}^{n} w_i f_i,\ f_i = f(x_i)$$

- In method of moments there are $2(n+1)$ parameters, $n+1$ weights, $n+1$ $x_i$'s
- Can impose exact quadrature up to degree $2n+1$
- Consider $p_{2n+1}(t)$ a polynomial of degree $2n+1$

$$I_{\mathrm{ab}}(p) = \int_a^b \omega(t) p(t)\,\mathrm{d}t$$

- Introduce scalar product

$$(f, g)_\omega = \int_a^b \omega(t) f(t)\, g(t)\,\mathrm{d}t$$

with $\omega(t)$ assumed to satisfy scalar product properties ($t \in [a, b] \Rightarrow \omega(t) \geqslant 0$)

- Introduce $\varphi_k(t)$ polynomials orthogonal w.r.t. $(f, g)_\omega$ scalar product

$$(\varphi_j, \varphi_k)_\omega = \delta_{jk}$$

- $\varphi_k$ polynomials can be found by Gram-Schmidt algorithm applied to $\{1, t, \dots\}$
- Divide $p_{2n+1}(t)$ by $\varphi_{n+1}(t)$

$$p_{2n+1}(t) = q_n(t)\,\varphi_{n+1}(t) + r_n(t)$$

- Example $p(t) = 3t^3 - 2t^2 + t + 1$ divided by $\varphi_1(t) = t^2 + t + 1$, $p_3(t) = q_1(t)\,\varphi_2(t) + r_1(t)$, $q_1(t) = 3t - 5$, $r_1(t) = 3t + 6$

$$\begin{array}{r|llll}
 & 3t & -5 & & \\ \hline
t^2+t+1 & 3t^3 & -2t^2 & +t & +1 \\
 & 3t^3 & +3t^2 & +3t & \\ \cline{3-5}
 & & -5t^2 & -2t & +1 \\
 & & -5t^2 & -5t & -5 \\ \cline{4-5}
 & & & 3t & +6
\end{array}$$

- Integrate $p_{2n+1}$

$$\int_a^b \omega(t) p_{2n+1}(t)\,\mathrm{d}t = \int_a^b \omega(t) q_n(t)\,\varphi_{n+1}(t)\,\mathrm{d}t + \int_a^b \omega(t) r_n(t)\,\mathrm{d}t$$

- However, $\varphi_{n+1}$ orthogonal w.r.t. to all polynomials of degree at most $n \Rightarrow$

$$\int_a^b \omega(t) q_n(t)\,\varphi_{n+1}(t)\,\mathrm{d}t = 0$$

- Obtain

$$\int_a^b \omega(t) p_{2n+1}(t)\,\mathrm{d}t = \int_a^b \omega(t) r_n(t)\,\mathrm{d}t = \sum_{i=0}^{n} w_i\, r_n(x_i)$$

  implying that a formula that is exact for polynomials up to degree $n$ is also exact for $p_{2n+1}$ of degree $2n+1$.
- Gauss observation: the only values of $p_{2n+1}$ that arise are $p_{2n+1}(x_i)$. Can $x_i$ be chosen such that $r_n(x_i) = p_{2n+1}(x_i) = q_n(x_i)\,\varphi_{n+1}(x_i) + r_n(x_i)$? Yes!
- Choose evaluation point $x_i$ such that $\varphi_{n+1}(x_i) = 0$, roots of $\varphi_{n+1}$

- $I(f) = \int_{-1}^{1} f(t)\,\mathrm{d}t$, weight $\omega(t) = 1$, scalar product $(f, g) = \int_{-1}^{1} f(t)\, g(t)\,\mathrm{d}t$
- Orthogonal family of polynomials are the Legendre polynomials

$$\left\{1, t, \frac{1}{2}(3t^2 - 1), \frac{1}{2}(5t^3 - 3t), \frac{1}{8}(35t^4 - 30t^2 + 3), \ldots\right\}$$

- Gauss-Legendre quadrature formulas
  - GL2 $n + 1 = 2 \Rightarrow \varphi_2(t) = \frac{1}{2}(3t^2 - 1)$ with roots $x_0 = -\frac{1}{\sqrt{3}}$, $x_1 = \frac{1}{\sqrt{3}}$.

$$I(f) = \int_{-1}^{1} f(t)\,\mathrm{d}t \cong Q(f) = f(x_0) + f(x_1), w_0 = w_1 = 1,$$

    exact up to cubics $I(p_3) = Q(p_3)$
  - GL3 $n + 1 = 3 \Rightarrow \varphi_3(t) = \frac{1}{2}(5t^3 - 3t)$ with roots $x_{0,2} = -\frac{\sqrt{3}}{\sqrt{35}}, x_1 = 0$,

$$\int_{-1}^{1} f(t)\,\mathrm{d}t \cong Q(f) = \frac{5}{9}f(x_0) + \frac{8}{9}f(x_1) + \frac{5}{9}f(x_2), w_0 = w_2 = \frac{5}{9}, w_1 = \frac{8}{9}$$

    exact up to quintics $I(p_5) = Q(p_5)$

- Gauss-Chebyshev sample points given by roots of $T_{n+1}(\theta) = \cos(n\theta)$, $x = \cos\theta$

$$x_i = \cos\frac{(2i+1)\pi}{2(n+1)}, i = 0, 1, 2, \ldots, n$$

- Gauss-Chebyshev weights are especially simple, they're all equal!

$$w_i = \frac{\pi}{n+1}$$

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}\, \mathrm{d}t \cong Q(f) = \sum_{i=0}^{n} w_i f_i, f_i = f(x_i)$$

- Relevant for Laplace transforms

$$\int_0^\infty e^{-t} f(t)\,\mathrm{d}t \cong Q(f) = \sum_{i=0}^{n} w_i f_i,\ f_i = f(x_i)$$

- Gauss-Laguerre 2, exact up to cubics

$$x_0 = 0.585786, w_0 = 0.853853, x_1 = 3.41421, w_1 = 0.146447$$

- Gauss-Laguerre 3, exact up to quintics

$$x_0 = 0.415775, w_0 = 0.711093, x_1 = 2.29428, w_1 = 0.278518$$

$$x_2 = 6.28995, w_2 = 0.0103893$$

- Relevant for Gauss distributions, diffusion equations

$$\int_{-\infty}^{\infty} e^{-t^2} f(t)\,\mathrm{d}t \cong Q(f) = \sum_{i=0}^{n} w_i f_i,\ f_i = f(x_i)$$

- Gauss-Hermite 2, exact up to cubics

$$x_{0,1} = \pm 0.707107,\ w_{0,1} = 0.886227$$

- Gauss-Hermite 3, exact up to quintics

$$x_{0,2} = \pm 1.22474,\ w_{0,1} = 0.0813128,\ x_1 = 0,\ w_1 = 1.18164$$

- Wiener transform $F(x)$ of $f(y)$ is

$$F(x) = \frac{1}{\sqrt{4\pi}} \int_{-\infty}^{\infty} e^{-(x-y)^2/4} f(y)\,\mathrm{d}y$$

specifies the temperature after one unit of time of a bar whose initial temperature was $f(y)$.