Chapter 3 Numerical Integration

3.1 Newton-Côtes Quadrature

- We want to calculate integration $\int_{\mathcal{X}} g(x)\,dx$ for some function $g(x)$ defined on $\mathcal{X} \subset \mathbb{R}$.
  - Let $f_X(x)$ be the PDF of random variable X, we may want to know

    $$F_X(x) = P(X \leq x) = \int_{-\infty}^{x} f_X(u)\,du$$

    or

    $$E\big[h(X)\big] = \int_{-\infty}^{\infty} h(x) f_X(x)\,dx.$$

  - Let $f_{XY}(x, y)$ be the joint PDF of (X, Y), we often need to calculate $f_Y(y) = \int_{-\infty}^{\infty} f_{XY}(x, y)\,dx$.

3.1 Newton-Côtes Quadrature

- **Bayesian Inference:** In Bayesian approaches, the parameter $\boldsymbol{\theta}$ is considered as a random variable.
  - Suppose $\boldsymbol{\theta}$ has a *prior distribution* with PDF $\pi(\theta)$. Given $\boldsymbol{\theta} = \theta$, the observed data X follows a distribution with PDF $f_{X|\boldsymbol{\theta}}(x|\theta)$.
  - The distribution of $\boldsymbol{\theta}$ conditional on the the observed data is called the *posterior distribution* of the parameter $\boldsymbol{\theta}$.
  - Let $f_{\theta|X}(\theta|x)$ be the PDF of the posterior distribution of $\boldsymbol{\theta}$. Then

$$f_{\boldsymbol{\theta}|X}(\theta|x) = \frac{f_{X\boldsymbol{\theta}}(x,\theta)}{f_X(x)} = \frac{f_{X\boldsymbol{\theta}}(x,\theta)}{\int f_{X\boldsymbol{\theta}}(x,\theta)\,d\theta} = \frac{\pi(\theta)f_{X|\boldsymbol{\theta}}(x|\theta)}{\int \pi(\theta)f_{X|\boldsymbol{\theta}}(x|\theta)\,d\theta}.$$

  - Suppose we want to calculate the probability $P(a < \boldsymbol{\theta} < b|X = x)$, then

$$P(a < \boldsymbol{\theta} < b|X = x) = \int_a^b f_{\boldsymbol{\theta}|X}(\theta|x)\,d\theta = \frac{\int_a^b \pi(\theta)f_{X|\boldsymbol{\theta}\,d\theta}(x|\theta)\,d\theta}{\int \pi(\theta)f_{X|\boldsymbol{\theta}}(x|\theta)\,d\theta}.$$

- **Example:** Suppose that $X_1, \cdots, X_n$ are i.i.d. from the Poisson(θ) distribution given that $\boldsymbol{\theta} = \theta > 0$. Assume that the prior distribution of θ has the PDF $\pi(\theta) = \frac{1}{\Gamma(\alpha)\beta^\alpha}\theta^{\alpha-1}e^{-\theta/\beta}$, $\theta > 0$ (the Gamma(α, β) distribution with $\alpha > 0$ and $\beta > 0$), where $\Gamma(\alpha) = \int_0^\infty t^{\alpha-1}e^{-t}dt$.
  - The distribution of $X_1 = x_1, \cdots, X_n = x_n$ given $\boldsymbol{\theta} = \theta$ is

$$P\big(X_1 = x_1, \cdots, X_n = x_n | \boldsymbol{\theta} = \theta\big) = \prod_{i=1}^n P\big(X_i = x_i | \boldsymbol{\theta} = \theta\big) = \frac{e^{-n\theta}\,\theta^{\sum_{i=1}^n x_i}}{\prod_{i=1}^n x_i!}.$$

  - The posterior distribution of $\boldsymbol{\theta}$ is

$$\begin{aligned} f_{\boldsymbol{\theta}|X}(\theta \mid X = x) &= \frac{\pi(\theta)P(X_1 = x_1, \cdots, X_n = x_n \mid \boldsymbol{\theta} = \theta)}{\int_\Theta \pi(\theta)P(X_1 = x_1, \cdots, X_n = x_n \mid \boldsymbol{\theta} = \theta)d\theta} \\ &= \frac{\frac{1}{\Gamma(\alpha)\beta^\alpha}\theta^{\alpha-1}e^{-\theta/\beta}}{\int_\Theta \pi(\theta)P(X_1 = x_1, \cdots, X_n = x_n \mid \boldsymbol{\theta} = \theta)d\theta} \cdot \frac{e^{-n\theta}\,\theta^{\sum_{i=1}^n x_i}}{\prod_{i=1}^n x_i!} \\ &= c(x_1, \cdots, x_n) \cdot \theta^{\alpha+\sum_{i=1}^n x_i - 1}\, e^{-(n\beta+1)\theta/\beta}, \end{aligned}$$

    which is the Gamma($\alpha + \sum_{i=1}^n x_i$, $\frac{\beta}{n\beta+1}$) distribution.

3.1 Newton-Côtes Quadrature

- When $\int_{-\infty}^{\infty} g(x)\,dx$ exists, we have $\int_a^b g(x)\,dx \to \int_{-\infty}^{\infty} g(x)\,dx$. when $a \to -\infty$ and $b \to \infty$. So we can choose $a < b$ so that $\int_a^b g(x)\,dx \approx \int_{-\infty}^{\infty} g(x)\,dx$. We focus on calculate $\int_a^b g(x)\,dx$ in the following.

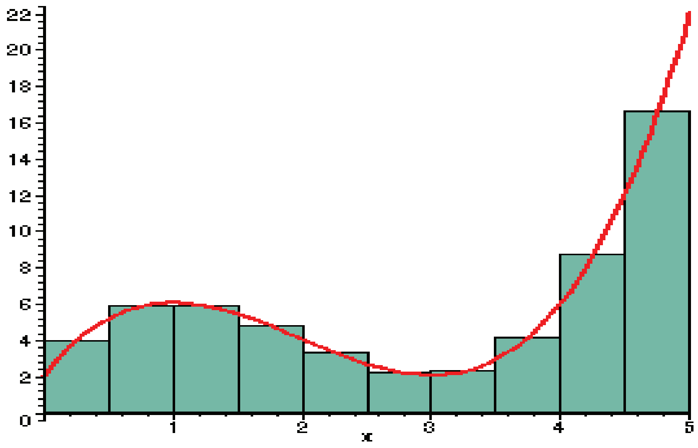
- **Riemann Rule:** Let $a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b$ be a partition of interval $[a, b]$ and let ξ_i be any point between x_i and x_{i+1}. Then

$$\sum_{i=0}^{n-1} g(\xi_i)(x_{i+1} - x_i) \to \int_a^b g(x)\,dx$$

  as $\max\left\{|x_1 - x_0|, \cdots, |x_n - x_{n-1}|\right\} \to 0$.

  - Assume that $x_0, x_1, \cdots, x_n$ are equally spaced in the following. That is, $x_i = a + i(b-a)/n$ for $i = 0, 1, \cdots, n$.
  - For simplicity, we use h_n to denote $(b-a)/n$ in the following.

3.1 Newton-Côtes Quadrature



- – If we let $\xi_i = x_i$, then $\int_a^b g(x)\,dx$ is estimated by

$$R_{1,n} = h_n \sum_{i=0}^{n-1} g(x_i).$$

  – If we let $\xi_i = (x_i + x_{i+1})/2$, then $\int_a^b g(x)\,dx$ is estimated by

$$R_{2,n} = h_n \sum_{i=0}^{n-1} g\big((x_i + x_{i+1})/2\big).$$

- – We say $a_n = O(b_n)$ if we can find $c > 0$ such that $|a_n/b_n| < c$ for all n, and $a_n = o(b_n)$ if $\lim_{n\to\infty} a_n/b_n = 0$.

  – Assume that $g''(x)$ is continuous on [a,b]. For $R_{1,n}$, we have

$$\begin{aligned}
&\left|R_{1,n} - \int_a^b g(x)\,dx\right| \\
= &\left|h_n \sum_{i=0}^{n-1} g(x_i) - \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} g(x)\,dx\right| \le \sum_{i=0}^{n-1} \left|h_n g(x_i) - \int_{x_i}^{x_{i+1}} g(x)\,dx\right| \\
= &\sum_{i=0}^{n-1} \left|h_n g(x_i) - \int_{x_i}^{x_{i+1}} \left[g(x_i) + g'(x_i)(x - x_i) + \frac{1}{2} g''(u_i)(x - x_i)^2\right] dx\right| \\
= &\sum_{i=0}^{n-1} \left| - \frac{1}{2} g'(x_i) h_n^2 - \int_{x_i}^{x_{i+1}} \frac{1}{2}\, g''(u_i)(x - x_i)^2\, dx\right| \\
\le &\; c \sum_{i=0}^{n-1} h_n^2 = O(h_n) = O(1/n),
\end{aligned}$$

  where u_i is a point between x and x_i.

- – For $R_{2,n}$, we have

$$\left|R_{2,n} - \int_a^b g(x)\,dx\right| = \left|h_n \sum_{i=0}^{n-1} g\left(\frac{x_i + x_{i+1}}{2}\right) - \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} g(x)\,dx\right|$$

$$\leq \sum_{i=0}^{n-1} \left|h_n g\left(\frac{x_i + x_{i+1}}{2}\right) - \int_{x_i}^{x_{i+1}} g(x)\,dx\right|$$

$$= \sum_{i=0}^{n-1} \left|h_n g\left(\frac{x_i + x_{i+1}}{2}\right) - \int_{x_i}^{x_{i+1}} \left[g\left(\frac{x_i + x_{i+1}}{2}\right) + g'\left(\frac{x_i + x_{i+1}}{2}\right) \cdot \left(x - \frac{x_i + x_{i+1}}{2}\right)\right.\right.$$

$$\left.\left. + \frac{1}{2} g''(u_i) \cdot \left(x - \frac{x_i + x_{i+1}}{2}\right)^2 \right] dx\right|$$

$$= \sum_{i=0}^{n-1} \left|0 - \int_{x_i}^{x_{i+1}} \frac{1}{2} g''(u_i) \cdot \left(x - \frac{x_i + x_{i+1}}{2}\right)^2]\,dx\right|$$

$$\leq c \sum_{i=0}^{n-1} h_n^3 = O(h_n^2) = O(1/n^2).$$

  – Hence, $R_{2,n}$ converges faster than $R_{1,n}$.

3.1 Newton-Côtes Quadrature

- **Newton-Côtes Quadrature:** The Newton-Côtes quadrature proposes to use a mth degree polynomial (**instead of a constant**) to approximate $g(x)$ in each subinterval $[x_i, x_{i+1}]$, $i = 1, \cdots, n$.
  - We insert $m-1$ equally spaced points in the interval $[x_i, x_{i+1}]$. Define $x^*_{ij} = x_i + jh_n/m$, $j = 0, \cdots, m$. Then $x^*_{i0} = x_i$ and $x^*_{im} = x_{i+1}$.
  - Define
$$p_{ij}(x) = \prod_{k=0,k\neq j}^{m} \frac{x - x^*_{ik}}{x^*_{ij} - x^*_{ik}}.$$
It is easy to find that $p_{ij}(x)$ is a mth degree polynomial, $p_{ij}(x^*_{ij}) = 1$ and $p_{ij}(x^*_{ik}) = 0$ for $k = 0, \cdots, m$ and $k \neq j$.
  - Let $\hat{g}_i(x) = \sum_{j=0}^{m} g(x^*_{ij}) p_{ij}(x)$. Then $\hat{g}_i(x)$ is a mth degree polynomial, and it satisfies $\hat{g}_i(x^*_{ij}) = g(x^*_{ij})$ for $j = 0, \cdots, m$.

3.1 Newton-Côtes Quadrature

- – The Newton-Côtes quadrature proposes to calculate $\int_a^b g(x)\,dx$ by

$$\begin{aligned}\int_a^b g(x)\,dx &= \sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}} g(x)\,dx \\ &\approx \sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}} \hat{g}_i(x)\,dx = \sum_{i=0}^{n-1}\sum_{j=0}^{m} g(x_{ij}^*)\int_{x_i}^{x_{i+1}} p_{ij}(x)\,dx.\end{aligned}$$

  – When $m = 1$, we have $x_{i0}^* = x_i$, $x_{i1}^* = x_{i+1}$ and $p_{i0}(x) = \frac{x-x_{i+1}}{x_i-x_{i+1}}$, $p_{i1}(x) = \frac{x-x_i}{x_{i+1}-x_i}$. Note that $x_{i+1} - x_i = h_n$, we have

$$\int_{x_i}^{x_{i+1}} p_{i0}(x)\,dx = \frac{h_n}{2} \quad \text{and} \quad \int_{x_i}^{x_{i+1}} p_{i1}(x)\,dx = \frac{h_n}{2}.$$

  Then $\int_a^b g(x)\,dx$ is estimated by

$$T_n = \sum_{i=0}^{n-1}\left[\frac{h_n}{2}g(x_i) + \frac{h_n}{2}g(x_{i+1})\right] = \frac{h_n}{2}g(x_0) + h_n\sum_{i=1}^{n-1} g(x_i) + \frac{h_n}{2}g(x_n).$$

  This method is called the *trapezoidal rule*.

- – When $m = 2$, $x_{i0}^* = x_i$, $x_{i1}^* = (x_i + x_{i+1})/2$, and $x_{i2}^* = x_{i+1}$. We can show that **(Homework)**

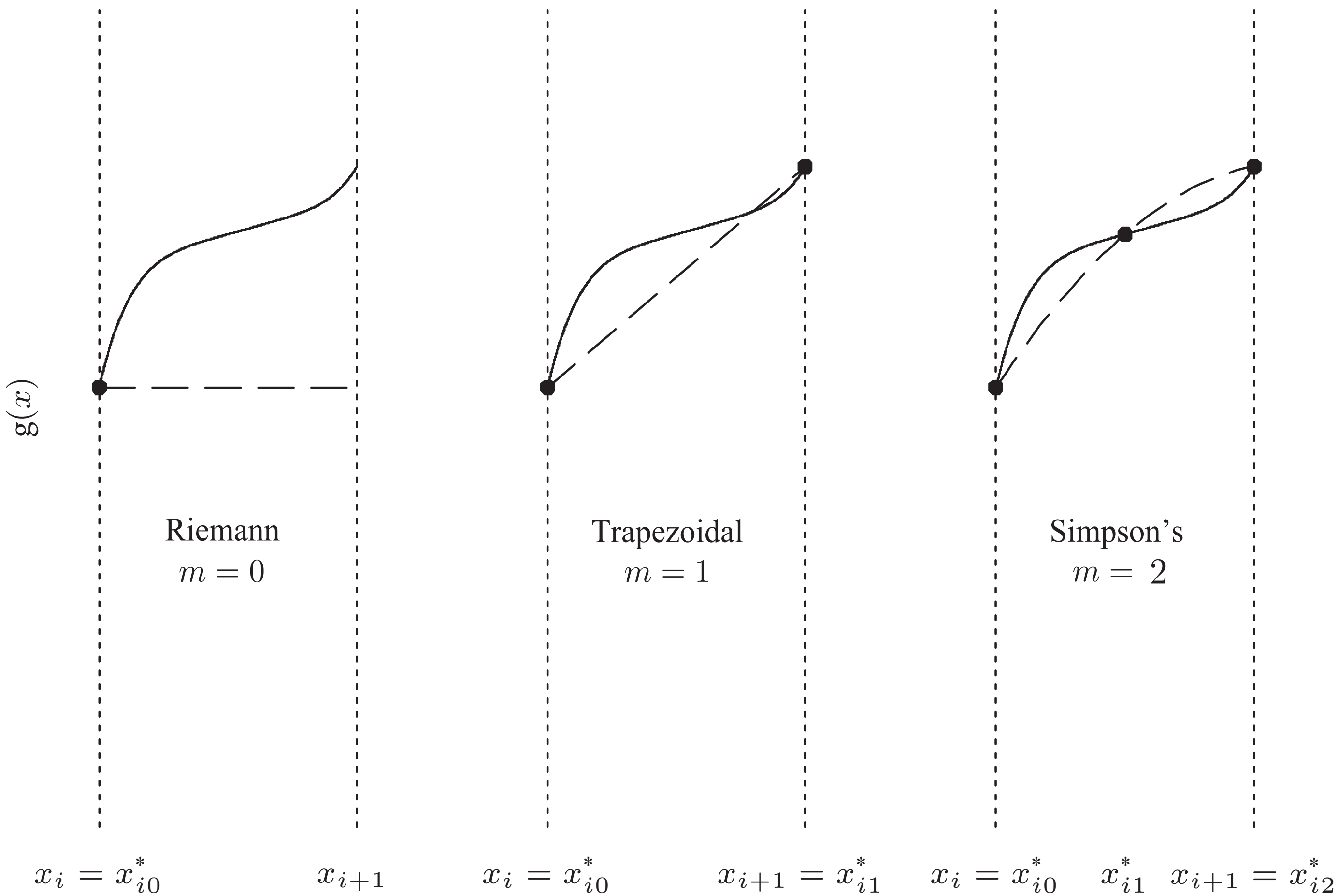
  $$\int_{x_i}^{x_{i+1}} p_{i0}(x)\,dx = \int_{x_i}^{x_{i+1}} p_{i2}(x)\,dx = \frac{h_n}{6} \quad \text{and} \quad \int_{x_i}^{x_{i+1}} p_{i1}(x)\,dx = \frac{2h_n}{3}.$$

  Then $\int_a^b g(x)\,dx$ is estimated by

  $$\begin{aligned} S_n &= \sum_{i=0}^{n-1} \Big[\frac{h_n}{6} g(x_i) + \frac{2h_n}{3} g\Big(\frac{x_i + x_{i+1}}{2}\Big) + \frac{h_n}{6} g(x_{i+1})\Big] \\ &= \frac{h_n}{6} g(x_0) + \frac{h_n}{3} \sum_{i=1}^{n-1} g(x_i) + \frac{2h_n}{3} \sum_{i=0}^{n-1} g\Big(\frac{x_i + x_{i+1}}{2}\Big) + \frac{h_n}{6} g(x_n). \end{aligned}$$

  This method is called the *Simpson's rule.*

3.1 Newton-Côtes Quadrature



Riemann Rule, trapezoidal rule and Simpson's rule

- Next, we consider the convergence rates of different rules.

- **Bernoulli Polynomials:** The *Bernoulli polynomials* $\{B_k(x), 0 \le x \le 1\}$ are defined recursively by $B_0(x) = 1$, and for $k \ge 1$,

$$B_k'(x) = kB_{k-1}(x) \quad \text{and} \quad \int_0^1 B_k(x)\,dx = 0.$$

- **Remarks:**

  – By definition, we have $B_1(x) = x - 1/2$, $B_2(x) = x^2 - x + 1/6$, $\cdots$

  – Each $B_k(x)$ is a polynomial of order k. We need the condition $\int_0^1 B_k(x)\,dx = 0$ to determine the constant term in the polynomial.

  – Note that by definition,

$$\big[B_{k+1}(1) - B_{k+1}(0)\big] = (k+1)\int_0^1 B_k(x)\,dx.$$

  The condition $\int_0^1 B_k(x)\,dx = 0$ guarantees that $B_{k+1}(1) = B_{k+1}(0)$ for $k = 1, 2, \cdots$.

3.1 Newton-Côtes Quadrature

- **Eular-Maclaurin Formula:** Let $m < n$ be two integers and let $g(x)$ be a p-times continuously differentiable function on the interval $[m, n]$. Then

$$\sum_{i=m+1}^{n} g(i) \;=\; \int_m^n g(x)\,dx + \frac{g(n)-g(m)}{2} + \sum_{k=1}^{p-1} \frac{(-1)^{k+1}B_{k+1}(0)}{(k+1)!}\big(g^{(k)}(n) - g^{(k)}(m)\big)$$
$$+(-1)^{p+1}\sum_{i=m+1}^{n}\int_{i-1}^{i}\frac{g^{(p)}(x)}{p!}\,B_p(x+1-i)\,dx.$$

- **Proof.**

  – We first consider $\int_{i-1}^{i} g(x)\,dx$ for $i = m+1, \cdots, n$. Then

$$\begin{aligned}
\int_{i-1}^{i} g(x)\,dx &= \int_{i-1}^{i} g(x)\,d(x-i+1/2) \\
&= g(x)(x-i+1/2)\Big|_{x=i-1}^{i} - \int_{i-1}^{i}(x-i+1/2)\,dg(x) \\
&= \frac{g(i)+g(i-1)}{2} - \int_{i-1}^{i} B_1(x+1-i)g'(x)\,dx.
\end{aligned}$$

3.1 Newton-Côtes Quadrature

- – Thus, we have

$$\begin{aligned}
g(i) &= \int_{i-1}^{i} g(x)\,dx + \frac{g(i)-g(i-1)}{2} + \int_{i-1}^{i} B_1(x+1-i)g'(x)\,dx \\
&= \int_{i-1}^{i} g(x)\,dx + \frac{g(i)-g(i-1)}{2} + \int_{i-1}^{i} g'(x)dB_2(x+1-i)/2 \\
&= \int_{i-1}^{i} g(x)\,dx + \frac{g(i)-g(i-1)}{2} + \frac{g'(i)B_2(1)-g'(i-1)B_2(0)}{2!} - \frac{1}{2}\int_{i-1}^{i} B_2(x+1-i)g''(x)dx \\
&= \int_{i-1}^{i} g(x)\,dx + \frac{g(i)-g(i-1)}{2} + \frac{B_2(0)}{2!}\big(g'(i)-g'(i-1)\big) - \frac{1}{2}\int_{i-1}^{i} B_2(x+1-i)g''(x)dx \\
&= \cdots\cdots \\
&= \int_{i-1}^{i} g(x)\,dx + \frac{g(i)-g(i-1)}{2} + \sum_{k=1}^{p-1} \frac{(-1)^{k+1}B_{k+1}(0)}{(k+1)!}\big(g^{(k)}(i)-g^{(k)}(i-1)\big) \\
&\qquad + (-1)^{p+1}\int_{i-1}^{i} \frac{g^{(p)}(x)}{p!} B_p(x+1-i)\,dx.
\end{aligned}$$

  – Take sum of both sides for $i = m+1, \cdots, n$, we obtain

$$\begin{aligned}
\sum_{i=m+1}^{n} g(i) &= \int_{m}^{n} g(x)\,dx + \frac{g(n)-g(m)}{2} + \sum_{k=1}^{p-1} \frac{(-1)^{k+1}B_{k+1}(0)}{(k+1)!}\big(g^{(k)}(n)-g^{(k)}(m)\big) \\
&\qquad + (-1)^{p+1}\sum_{i=m+1}^{n}\int_{i-1}^{i} \frac{g^{(p)}(x)}{p!} B_p(x+1-i)\,dx.
\end{aligned}$$

3.1 Newton-Côtes Quadrature

- **Remarks:**
  - $B_k(0)$ are called *Bernoulli numbers*. The Bernoulli numbers from $B_1(0)$ to $B_7(0)$ are $\frac{1}{2}$, $\frac{1}{6}$, 0, $-\frac{1}{30}$, 0, $\frac{1}{42}$, 0.
  - We can show that $B_k(0)$**=0 for** k**=3,5,7,9,** $\cdots$.
  - The Eular-Maclaurin formula can also be written as

$$\sum_{i=m}^{n} g(i) = \int_m^n g(x)\,dx + \frac{g(n)+g(m)}{2} + \sum_{s=1}^{q} \frac{B_{2s}(0)}{(2s)!}\big(g^{(2s-1)}(n) - g^{(2s-1)}(m)\big)$$
$$+ \sum_{i=m+1}^{n} \int_{i-1}^{i} \frac{g^{(2q+1)}(x)}{p!}\, B_{2q+1}(x+1-i)\,dx.$$

3.1 Newton-Côtes Quadrature

- Now we consider $\int_a^b g(x)\,dx$ for $-\infty < a < b < \infty$. Set $x_i = a + \frac{i*(b-a)}{n}$ for $i = 0, 1, \cdots, n$. Then $a = x_0 < x_1 < \cdots < x_n = b$ forms a partition of the interval $[a, b]$.
  - Let $h_n = (b-a)/n$. Define $\varphi(u) = g(a + h_n u)$. It is easy to know that
    $$\int_a^b g(x)\,dx = \int_0^n g(a + h_n u)\,d(a + h_n u) = h_n \int_0^n \varphi(u)\,du.$$
  - Applying the Eular-Maclaurin formula to $\int_0^n \varphi(u)\,du$, we obtain

$$\begin{aligned}\int_a^b g(x)\,dx \;=\; & h_n \sum_{i=0}^{n} \varphi(i) - h_n \cdot \frac{\varphi(0)+\varphi(n)}{2} - h_n \cdot \sum_{s=1}^{q} \frac{B_{2s}(0)}{(2s)!}\big(\varphi^{(2s-1)}(n) - \varphi^{(2s-1)}(0)\big) \\ & -h_n \cdot \sum_{i=1}^{n} \int_{i-1}^{i} \frac{\varphi^{(2q+1)}(u)}{p!}\, B_{2q+1}(u+1-i)\,dx.\end{aligned}$$

- – Note that $\varphi(0) = g(a)$, $\varphi(i) = g(x_i)$, $\varphi(n) = g(b)$, $\varphi^{(k)}(u) = h_n^k g^{(k)}(a + h_n u)$. Then

$$\begin{aligned}
\int_a^b g(x)\,dx \;&=\; h_n \sum_{i=0}^{n} g(x_i) - h_n \cdot \frac{g(a)+g(b)}{2} \\
&\qquad - \sum_{s=1}^{q} h_n^{2s} \cdot \frac{B_{2s}(0)}{(2s)!}\Big(g^{(2s-1)}(b) - g^{(2s-1)}(a)\Big) + O(h_n^{2q+1}) \\
&=\; h_n \sum_{i=0}^{n} g(x_i) - h_n \cdot \frac{g(a)+g(b)}{2} - \frac{h_n^2}{12}\Big(g'(b) - g'(a)\Big) \\
&\qquad + \frac{h_n^4}{720}\Big(g^{(3)}(b) - g^{(3)}(a)\Big) - \frac{h_n^6}{720 \cdot 42}\Big(g^{(5)}(b) - g^{(5)}(a)\Big) + \cdots .
\end{aligned}$$

3.1 Newton-Côtes Quadrature

- Consider the convergence rates of different rules to estimate $\int_a^b g(x)\,dx$.
  - According to the Eular-Maclaurin formula, we have

$$\begin{aligned} h_n \sum_{i=0}^{n} g(x_i) \;&=\; \int_a^b g(x)\,dx + h_n \cdot \frac{g(a)+g(b)}{2} + \frac{h_n^2}{12}\big(g'(b) - g'(a)\big) \\ &\quad - \frac{h_n^4}{720}\big(g^{(3)}(b) - g^{(3)}(a)\big) + \frac{h_n^6}{720 \cdot 42}\big(g^{(5)}(b) - g^{(5)}(a)\big) + \cdots . \end{aligned}$$

  - For the Riemann rule,

$$\begin{aligned} R_{1,n} \;&=\; h_n \sum_{i=0}^{n-1} g(x_i) = h_n \sum_{i=0}^{n} g(x_i) - h_n g(b) \\ &=\; \int_a^b g(x)\,dx + h_n \cdot \frac{g(a)+g(b)}{2} + O(h_n^2) - h_n g(b) \\ &=\; \int_a^b g(x)\,dx + O(1/n). \end{aligned}$$

- – Note that $h_n = (b-a)/n$, so $h_n = 2 \cdot h_{2n}$. We have

$$\begin{aligned}
R_{2,n} &= h_n \sum_{i=0}^{n-1} g\big((x_i + x_{i+1})/2\big) \\
&= 2 \cdot h_{2n} \Big[\sum_{i=0}^{n} g(x_i) + \sum_{i=0}^{n-1} g\big((x_i + x_{i+1})/2\big) \Big] - h_n \sum_{i=0}^{n} g(x_i) \\
&= 2 \Big[\int_a^b g(x)\,dx + h_{2n} \cdot \frac{g(a)+g(b)}{2} + \frac{h_{2n}^2}{12}\big(g'(b) - g'(a)\big) + O(h_n^4) \Big] \\
&\qquad - \Big[\int_a^b g(x)\,dx + h_n \cdot \frac{g(a)+g(b)}{2} + \frac{h_n^2}{12}\big(g'(b) - g'(a)\big) + O(h_n^4) \Big] \\
&= \int_a^b g(x)\,dx - \frac{h_n^2}{24}\big(g'(b) - g'(a)\big) + O(h_n^4) \\
&= \int_a^b g(x)\,dx + O(1/n^2).
\end{aligned}$$

- – For the trapezoidal rule, we have

$$
\begin{aligned}
T_n &= \frac{h_n}{2} g(x_0) + h_n \sum_{i=1}^{n-1} g(x_i) + \frac{h_n}{2} g(x_n) \\
&= h_n \sum_{i=0}^{n} g(x_i) - h_n \cdot \frac{g(a)+g(b)}{2} \\
&= \int_a^b g(x)\,dx + h_n \cdot \frac{g(a)+g(b)}{2} + \frac{h_n^2}{12}\big(g'(b)-g'(a)\big) + O(h_n^4) - h_n \cdot \frac{g(a)+g(b)}{2}.
\end{aligned}
$$

  – For the Simpson's rule, we have

$$
\begin{aligned}
S_n &= \frac{h_n}{6} g(x_0) + \frac{h_n}{3} \sum_{i=1}^{n-1} g(x_i) + \frac{2h_n}{3} \sum_{i=0}^{n-1} g\Big(\frac{x_i + x_{i+1}}{2}\Big) + \frac{h_n}{6} g(x_n) \\
&= \frac{4}{3} \cdot h_{2n} \Big[\sum_{i=0}^{n} g(x_i) + \sum_{i=0}^{n-1} g\big((x_i + x_{i+1})/2\big) \Big] - \frac{h_n}{3} \sum_{i=0}^{n} g(x_i) \\
&\qquad - \frac{h_n}{3} \cdot \frac{g(a)+g(b)}{2}.
\end{aligned}
$$

3.1 Newton-Côtes Quadrature

- – Applying the Eular-Maclaurin formula, we have

$$
\begin{aligned}
S_n &= \frac{4}{3}\Big[\int_a^b g(x)\,dx + \frac{h_n}{2}\cdot\frac{g(a)+g(b)}{2} + \frac{h_n^2/4}{12}\big(g'(b)-g'(a)\big) + O(h_n^4)\Big] \\
&\qquad -\frac{1}{3}\Big[\int_a^b g(x)\,dx + h_n\cdot\frac{g(a)+g(b)}{2} + \frac{h_n^2}{12}\big(g'(b)-g'(a)\big) + O(h_n^4)\Big] \\
&\qquad\qquad -\frac{h_n}{3}\cdot\frac{g(a)+g(b)}{2} \\
&= \int_a^b g(x)\,dx + O(h_n^4) \\
&= \int_a^b g(x)\,dx + O(1/n^4).
\end{aligned}
$$

- **Choice of n:** Let Π_n be the Newton-Côtes quadrature estimates using n subintervals. In practice, we can choose n so that the relative error $\frac{|\Pi_n - \Pi_{n/2}|}{\Pi_{n/2}}$ is less than a given threshold value.

3.2 Gaussian Quadrature*

- In general, if we use $m+1$ equally spaced points $x_0, \cdots, x_m$, we can approximate $\int_a^b g(x)\,dx$ by $\sum_{i=0}^m a_i g(x_i)$, so that

$$\int_a^b g(x)\,dx = \sum_{i=0}^m a_i \cdot g(x_i)$$

whenever g is a polynomial of **degree not exceeding** m**.**

  – Define

$$\bar{p}_i(x) = \prod_{k=0,k\neq i}^m \frac{x-x_k}{x_i-x_k}.$$

Then $p_i(x_i) = 1$ and $p_i(x_k) = 0$ for $k = 0, \cdots, m$ and $k \neq i$.

  – Let

$$\hat{g}(x) = \sum_{i=0}^m g(x_i)\bar{p}_i(x).$$

We have that $\hat{g}(x)$ is a mth degree polynomial (its degree may be less than m), and it satisfies $\hat{g}(x_i) = g(x_i)$ for $j = 0, \cdots, m$.

3.2 Gaussian Quadrature*

- – Note that there is **only one** mth degree polynomial $p(\cdot)$ satisfying $p(x_i) = g(x_i)$ for $j = 0, \cdots, m$. If g is a also mth degree polynomial, we have $g(x) = \hat{g}(x)$ and

$$\int_a^b g(x)\,dx = \int_a^b \hat{g}(x)\,dx = \sum_{i=0}^{m} \int_a^b \bar{p}_i(x)\,dx \cdot g(x_i).$$

  – If the constraint of equally spaced points is removed, we can choose specially designed $x_0, x_1, \cdots, x_m$ so that the equality may hold for higher order polynomials.

3.2 Gaussian Quadrature*

- The *Gaussian quadrature* proposes to choose $x_0, \cdots, x_m$ so that

$$\int g(x)w(x)\,dx = \sum_{i=0}^{m} a_i \cdot g(x_i)$$

whenever g is a polynomial of **degree not exceeding** $2m+1$.

  – Here $w(x)$ is a nonnegative function and $\int |x^k| w(x)\,dx < \infty$ for $k \geq 0$.

  – When $w(x) = I(a \leq x \leq b)$, $\int g(x)w(x)\,dx = \int_a^b g(x)\,dx$.

  – When $w(x) = e^{-x} I(0 \leq x < \infty)$,

$$\int g(x)w(x)\,dx = \int_0^{\infty} g(x)e^{-x}\,dx = E\big[g(X)\big],$$

  where X follows an exponential distribution.

  – When $w(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$ for $-\infty < x < \infty$,

$$\int g(x)w(x)\,dx = \int_{-\infty}^{\infty} g(x)\frac{1}{\sqrt{2\pi}} e^{-x^2/2}\,dx = E\big[g(X)\big], \quad \text{where } X \sim N(0,1).$$

3.2 Gaussian Quadrature*

- **Orthogonal Polynomials:** Given nonnegative $w(x)$ satisfying $\int |x^k| w(x)\,dx < \infty$ for $k \geq 0$, we can find a series of polynomials $q_0(x)$, $q_1(x)$, $q_2(x)$, $\cdots$ that satisfy the following conditions.
  - Each $q_k(x)$ is a kth degree polynomial.
  - For $i \neq j$, $q_i(x)$ and q_j are *orthogonal* with respect to $w(x)$, that is

$$< q_i, q_j >_w := \int q_i(x) q_j(x) w(x)\,dx = 0.$$

- **Remark:** When $q_k(x)$ also satisfies $< q_k, q_k >_w = 1$ for all k, we call $q_0(x)$, $q_1(x)$, $q_2(x)$, $\cdots$ as *ortho-normal bases* with respect to $w(x)$.

3.2 Gaussian Quadrature*

- A orthogonal polynomials with respect to $w(x)$ can be constructed by applying the *Gram-Schmidt process* to $\{1, x, x^2, \cdots\}$. Specifically, we let $q_0(x) = 1$ and let

$$q_k(x) = x^k - \frac{< q_{k-1}, x^k >_w}{< q_{k-1}, q_{k-1} >_w} \cdot q_{k-1}(x) - \cdots - \frac{< q_0, x^k >_w}{< q_0, q_0 >_w} \cdot q_0(x).$$

  - When $w(x) = I(-1 \leq x \leq 1)$, the polynomials are called the *Legendre polynomials*.
  - When $w(x) = e^{-x} I(0 \leq x < \infty)$, the polynomials are called the *Laguerre polynomials*.
  - When $w(x) = e^{-x^2/2}$, the polynomials are called the *corrected Hermite polynomials*.

3.2 Gaussian Quadrature*

- **Gaussian Quadrature:** Given $w(x) \geq 0$ and $m > 0$, find the orthogonal polynomials $q_0(x), \cdots, q_{m+1}(x)$ with respect to $w(x)$.
  - Let $x_0 < x_1 < \cdots < x_m$ be the solutions of $q_{m+1}(x) = 0$.
  - We estimate $\int g(x)w(x)\, dx$ by
  $$\sum_{i=0}^{m} \int \bar{p}_i(x)w(x)\, dx \cdot g(x_i),$$
  where $\bar{p}_i(x) = \prod_{k=0,k\neq i}^{m} \frac{x-x_k}{x_i-x_k}$.

- **Remark:**
  - Here $x_0 < x_1 < \cdots < x_m$ and $\int \bar{p}_i(x)w(x)\, dx$ do not depend on g, they can be calculated in advance.
  - Usually, we will not use large m due to potential numerical imprecision introduced by computer roundoff error, for example, $m \leq 8$.

3.2 Gaussian Quadrature*

- – When g is a $(2m+1)$th degree polynomial, it can be written as

$$g(x) = s(x)q_{m+1}(x) + r(x),$$

where s and r are polynomials with degree not exceeding m.

* Note that $s(x) = b_m q_m(x) + \cdots + b_0 q_0(x)$ for some $b_0, \cdots, b_m$. Then

$$\int s(x)q_{m+1}(x)w(x)\,dx = 0.$$

* Since r is a polynomial with degree not exceeding m, we have

$$r(x) = \sum_{i=0}^{m} \bar{p}_i(x)r(x_i).$$

* Also note that $x_0 < x_1 < \cdots < x_m$ are the roots of $q_{m+1}(x)$. Hence,

$$g(x_i) = s(x_i)q_{m+1}(x_i) + r(x_i) = r(x_i).$$

- – * Finally, we have

$$
\begin{aligned}
\int g(x)w(x)\,dx &= \int \big[s(x)q_{m+1}(x) + r(x)\big]w(x)\,dx \\
&= \int r(x)w(x)\,dx \\
&= \int \Big[\sum_{i=0}^{m} \bar{p}_i(x)r(x_i)\Big]w(x)\,dx \\
&= \int \Big[\sum_{i=0}^{m} \bar{p}_i(x)g(x_i)\Big]w(x)\,dx \\
&= \sum_{i=0}^{m} \int \bar{p}_i(x)w(x)\,dx \cdot g(x_i).
\end{aligned}
$$

3.3 Frequently Encountered Problems

- **Range of Integration:** Consider integrals over infinite ranges.
  - We can choose $a < b$ so that $\int_a^b g(x)\,dx \approx \int_{-\infty}^{\infty} g(x)\,dx$.
  - We can also turn the infinite range to a finite range through one-to-one transformations. For example, we have

$$\begin{aligned}\int_{-\infty}^{\infty} g(x)\,dx &= \int_0^1 g\Big(\log\frac{u}{1-u}\Big)\,d\log\frac{u}{1-u}\\ &= \int_0^1 g\Big(\log\frac{u}{1-u}\Big)\cdot\frac{d\log\frac{u}{1-u}}{du}\,du\end{aligned}$$

  by letting $u = e^x/(1+e^x)$. Some other useful transformations include $1/x$, $x/(1+x)$ and $\exp\{-x\}$.

3.3 Frequently Encountered Problems

- **Multiple Integrals:** Consider calculation of $\int_a^b \int_c^d g(x,y)\,dydx$.
  - Define $x_i = a + i(b-a)/n$ for $i = 0, 1, \cdots, n$ and $y_j = c + j(d-c)/m$ for $j = 0, 1, \cdots, m$. Then

$$\int_a^b \int_c^d g(x,y)\,dydx \approx \frac{b-a}{n} \cdot \frac{d-c}{m} \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} g\left(\frac{x_i + x_{i+1}}{2}, \frac{y_j + y_{j+1}}{2}\right).$$

  - We can also consider $\int_c^d g(x,y)\,dy$ as $\varphi(x)$. Then

$$\int_a^b \int_c^d g(x,y)\,dydx = \int_a^b \varphi(x)\,dx \approx \sum_{i=0}^{n} a_i \cdot \varphi(x_i).$$

  We can use univariate quadrature approximations (*e.g.*, the Simpson's rule) to calculate $\varphi(x_i) = \int_c^d g(x_i, y)\,dy$ for each x_i.

Homework

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1. Suppose that $X_1, \cdots, X_n$ are i.i.d. from the $N(\theta, 4)$ distribution. Assume that the prior distribution of θ is $N(0, 10)$. Find the posterior distribution of θ given $X_1 = x_1, \cdots, X_n = x_n$.

2. To derive the Simpson's rule, prove that

$$\int_{x_i}^{x_{i+1}} p_{i0}(x)\,dx = \int_{x_i}^{x_{i+1}} p_{i2}(x)\,dx = \frac{h_n}{6} \quad \text{and} \quad \int_{x_i}^{x_{i+1}} p_{i1}(x)\,dx = \frac{2h_n}{3}.$$

3. Let X follow a Uniform$[1, 3]$ distribution. Compute $E\big(2/X\big) = \int_1^3 (1/x)\,dx$ using the Riemann rule (*i.e.*, $R_{1,n}$ and $R_{2,n}$), the trapezoidal rule (*i.e.*, T_n) and the Simpsons rule (*i.e.*, $S_{n/2}$) with $n = 4, 8, 16, 32, 64$. Discuss your results.

4. Suppose that X is from the $N(\mu, 9/7)$ distribution and assume that the prior distribution of $\boldsymbol{\mu}$ is the Cauchy(5,2) distribution with density $f_{\boldsymbol{\mu}}(\mu) = \frac{1}{2\pi\left[1+\left(\frac{\mu-5}{2}\right)^2\right]}$ for $-\infty < \mu < \infty$. Assume that $X = 5.3871$ is observed.
   (a) Using a numerical integration method of your choice, show that the proportionality constant k is roughly 7.84654. (In other words, find k such that $k \times \int$ (prior) $\times$ (likelihood) $d\mu = 1$.)
   (b) Using the value 7.84654 from (a), determine the posterior probability that $2 \le \mu \le 8$ using the Riemann rule (*i.e.*, $R_{1,n}$ and $R_{2,n}$), the trapezoidal rule (*i.e.*, T_n) and the Simpsons rule (*i.e.*, $S_{n/2}$). Compute the estimates until relative error within 0.0001 is achieved for the slowest method. Table the results.

Homework

4. (c) Use the transformation $u = 1/\mu$ to calculate the posterior probability that $\mu > 3$.