

Statistical Models & Computing Methods

Lecture 4: Numerical Integration



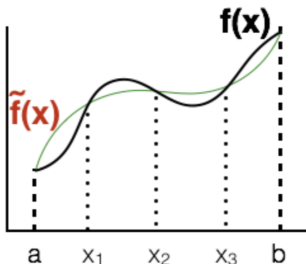
Cheng Zhang

School of Mathematical Sciences, Peking University

September 23, 2024

- ▶ Statistical inference often depends on intractable integrals
$$I(f) = \int_{\Omega} f(x)dx$$
- ▶ This is especially true in Bayesian statistics, where a posterior distribution is usually non-trivial.
- ▶ In some situations, the likelihood itself may depend on intractable integrals so frequentist methods would also require numerical integration
- ▶ In this lecture, we start by discussing some simple numerical methods that can be easily used in low dimensional problems
- ▶ Next, we will discuss several Monte Carlo strategies that could be implemented even when the dimension is high

- ▶ Consider a one-dimensional integral of the form
$$I(f) = \int_a^b f(x)dx$$
- ▶ A common strategy for approximating this integral is to use a tractable approximating function $\tilde{f}(x)$ that can be integrated easily
- ▶ We typically constrain the approximating function to agree with f on a grid of points: x_1, x_2, \dots, x_n



- ▶ Newton-Côtes methods use equally-spaced grids
- ▶ The approximating function is a polynomial
- ▶ The integral then is approximated with a weighted sum as follows

$$\hat{I} = \sum_{i=1}^n w_i f(x_i)$$

- ▶ In its simplest case, we can use the Riemann rule by partitioning the interval $[a, b]$ into n subintervals of length $h = \frac{b-a}{n}$; then

$$\hat{I}_L = h \sum_{i=0}^{n-1} f(a + ih)$$

This is obtained using a piecewise constant function \tilde{f} that matches f at the left points of each subinterval



- ▶ Alternatively, the approximating function could agree with the integrand at the right or middle point of each subinterval

$$\hat{I}_R = h \sum_{i=1}^n f(a + ih), \quad \hat{I}_M = h \sum_{i=0}^{n-1} f\left(a + \left(i + \frac{1}{2}\right)h\right)$$

- ▶ In either case, the approximating function is a zero-order polynomial
- ▶ To improve the approximation, we can use the trapezoidal rule by using a piecewise linear function that agrees with $f(x)$ at both ends of subintervals

$$\hat{I} = \frac{h}{2}f(a) + h \sum_{i=1}^{n-1} f(x_i) + \frac{h}{2}f(b)$$



- ▶ We would further improve the approximation by using higher order polynomials
- ▶ Simpson's rule uses a quadratic approximation over each subinterval

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{x_{i+1} - x_i}{6} \left(f(x_i) + 4f\left(\frac{x_i + x_{i+1}}{2}\right) + f(x_{i+1}) \right)$$

- ▶ In general, we can use any polynomial of degree k

- ▶ Newton-Côtes rules require equally spaced grids
- ▶ With a suitably flexible choice of $n + 1$ nodes, x_0, x_1, \dots, x_n , and corresponding weights, A_0, A_1, \dots, A_n ,

$$\sum_{i=0}^n A_i f(x_i)$$

gives the exact integration for all polynomials with degree less than or equal to $2n + 1$

- ▶ This is called **Gaussian** quadrature, which is especially useful for the following type of integrals $\int_a^b f(x)w(x)dx$ where $w(x)$ is a nonnegative function and $\int_a^b x^k w(x)dx < \infty$ for all $k \geq 0$

- ▶ In general, for squared integrable functions,

$$\int_a^b f(x)^2 w(x) dx \leq \infty$$

denoted as $f \in \mathcal{L}_{w,[a,b]}^2$, we define the inner product as

$$\langle f, g \rangle_{w,[a,b]} = \int_a^b f(x)g(x)w(x)dx$$

where $f, g \in \mathcal{L}_{w,[a,b]}^2$

- ▶ We said two functions to be *orthogonal* if $\langle f, g \rangle_{w,[a,b]} = 0$. If f and g are also scaled so that $\langle f, f \rangle_{w,[a,b]} = 1$, $\langle g, g \rangle_{w,[a,b]} = 1$, then f and g are orthonormal



- ▶ We can define a sequence of orthogonal polynomials by a recursive rule

$$T_{k+1}(x) = (\alpha_{k+1} + \beta_{k+1}x)T_k(x) - \gamma_{k+1}T_{k-1}(x)$$

- ▶ Example: Chebyshev polynomials (first kind).

$$T_0(x) = 1, \quad T_1(x) = x$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

- ▶ $T_n(x)$ are orthogonal with respect to $w(x) = \frac{1}{\sqrt{1-x^2}}$ and $[-1, 1]$

$$\int_{-1}^1 T_n(x)T_m(x) \frac{1}{\sqrt{1-x^2}} dx = 0, \quad \forall n \neq m$$



- ▶ In general orthogonal polynomials are not unique since $\langle f, g \rangle = 0$ implies $\langle cf, dg \rangle = 0$
- ▶ To make the orthogonal polynomial unique, we can use the following standardizations
 - ▶ make the polynomial orthonormal: $\langle f, f \rangle = 1$
 - ▶ set the leading coefficient of $T_j(x)$ to 1
- ▶ Orthogonal polynomials form a basis for $\mathcal{L}_{w,[a,b]}^2$ so any function in this space can be written as

$$f(x) = \sum_{n=0}^{\infty} a_n T_n(x)$$

$$\text{where } a_n = \frac{\langle f, T_n \rangle}{\langle T_n, T_n \rangle}$$



- ▶ Let $\{T_n(x)\}_{n=0}^{\infty}$ be a sequence of orthogonal polynomials with respect to w on $[a, b]$.
- ▶ Denote the $n + 1$ roots of $T_{n+1}(x)$ by

$$a < x_0 < x_1 < \dots < x_n < b.$$

- ▶ We can find weights A_1, A_2, \dots, A_{n+1} such that

$$\int_a^b P(x)w(x)dx = \sum_{i=0}^n A_i P(x_i), \quad \forall \deg(P) \leq 2n + 1$$

- ▶ To do that, we first show: there exists weights A_1, A_2, \dots, A_{n+1} such that

$$\int_a^b P(x)w(x)dx = \sum_{i=0}^n A_i P(x_i), \quad \forall \deg(P) < n + 1$$



- Sketch of proof. We only need to satisfy

$$\int_a^b x^k w(x) dx = \sum_{i=0}^n A_i x_i^k, \quad \forall k = 0, 1, \dots, n$$

This leads to a system of linear equations

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_0 & x_1 & \dots & x_n \\ \vdots & \vdots & \vdots & \vdots \\ x_0^n & x_1^n & \dots & x_n^n \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ \vdots \\ A_n \end{bmatrix} = \begin{bmatrix} I_0 \\ I_1 \\ \vdots \\ I_n \end{bmatrix}$$

where $I_k = \int_a^b x^k w(x) dx$. The determinant of the coefficient matrix is a Vandermonde determinant, and is non-zero since $x_i \neq x_j, \forall i \neq j$

- ▶ Now we show that the above Gaussian Quadrature can be exact for polynomials of degree $\leq 2n + 1$
- ▶ Let $P(x)$ be a polynomial with $\deg(P) \leq 2n + 1$, there exist polynomials $g(x)$ and $r(x)$ such that

$$P(x) = g(x)T_{n+1}(x) + r(x)$$

with $\deg(g) \leq n, \deg(r) \leq n$, Therefore,

$$\begin{aligned}\int_a^b P(x)w(x)dx &= \int_a^b r(x)w(x)dx = \sum_{i=0}^n A_i r(x_i) \\ &= \sum_{i=0}^n A_i P(x_i)\end{aligned}$$



- ▶ We now discuss the Monte Carlo method mainly in the context of statistical inference
- ▶ As before, suppose we are interested in estimating $I(h) = \int_a^b h(x)dx$
- ▶ If we can draw iid samples, $x^{(1)}, x^{(2)}, \dots, x^{(n)}$ uniformly from (a, b) , we can approximate the integral as

$$\hat{I}_n = (b - a) \frac{1}{n} \sum_{i=1}^n h(x^{(i)})$$

- ▶ Note that we can think about the integral as

$$(b - a) \int_a^b h(x) \cdot \frac{1}{b - a} dx$$

where $\frac{1}{b-a}$ is the density of $\text{Uniform}(a, b)$



- ▶ In general, we are interested in integrals of the form $\int_{\mathcal{X}} h(x)f(x)dx$, where $f(x)$ is a probability density function
- ▶ Analogous to the above argument, we can approximate this integral (or expectation) by drawing iid samples $x^{(1)}, x^{(2)}, \dots, x^{(n)}$ from the density $f(x)$ and then

$$\hat{I} = \frac{1}{n} \sum_{i=1}^n h(x^{(i)})$$

- ▶ Based on the law of large numbers, we know that

$$\lim_{n \rightarrow \infty} \hat{I}_n \xrightarrow{p} I$$

- ▶ And based on the central limit theorem

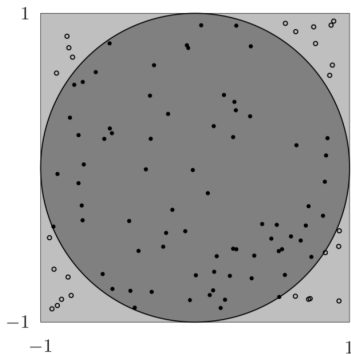
$$\sqrt{n}(\hat{I}_n - I) \rightarrow \mathcal{N}(0, \sigma^2), \quad \sigma^2 = \text{Var}(h(X))$$



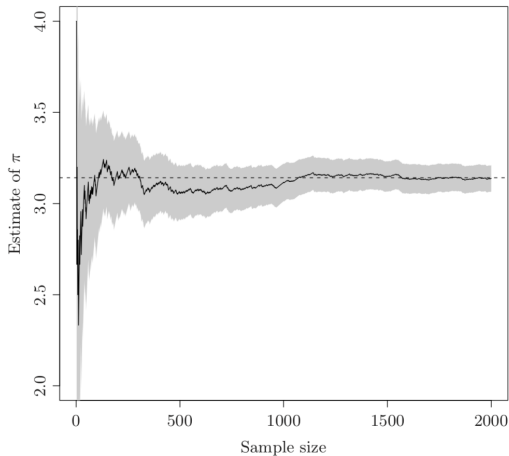
- ▶ Let $h(x) = \mathbf{1}_{B(0,1)}(x)$, then $\pi = 4 \int_{[-1,1]^2} h(x) \cdot \frac{1}{4} dx$
- ▶ Monte Carlo estimate of π

$$\hat{I}_n = \frac{4}{n} \sum_{i=1}^n \mathbf{1}_{B(0,1)}(x^{(i)})$$

$$x^{(i)} \sim \text{Uniform}([-1, 1]^2)$$



Monte Carlo estimate of π (with 90% confidence interval)



- ▶ Convergence rate for Monte Carlo: $\mathcal{O}(n^{-1/2})$

$$p\left(|\hat{I}_n - I| \leq \frac{\sigma}{\sqrt{n\delta}}\right) \geq 1 - \delta, \quad \forall \delta$$

often slower than quadrature methods ($\mathcal{O}(n^{-2})$ or better)

- ▶ However, the convergence rate of Monte Carlo does not depend on dimensionality
- ▶ On the other hand, quadrature methods are difficult to extend to multidimensional problems, because of the curse of dimensionality. The actual convergence rate becomes $\mathcal{O}(n^{-k/d})$, for any order k method in dimension d
- ▶ This makes Monte Carlo strategy very attractive for high dimensional problems



- ▶ Monte Carlo methods require sampling a set of points chosen randomly from a probability distribution
- ▶ For simple distribution $f(x)$ whose inverse cumulative distribution functions (CDF) exists, we can sampling x from f as follows

$$x = F^{-1}(u), \quad u \sim \text{Uniform}(0, 1)$$

where F^{-1} is the inverse CDF of f

- ▶ Proof.

$$p(a \leq x \leq b) = p(F(a) \leq u \leq F(b)) = F(b) - F(a)$$



- ▶ Exponential distribution: $f(x) = \theta \exp(-\theta x)$. The CDF is

$$F(a) = \int_0^a \theta \exp(-\theta x) = 1 - \exp(-\theta a)$$

therefore, $x = F^{-1}(u) = -\frac{1}{\theta} \log(1 - u) \sim f(x)$. Since $1 - u$ also follows the uniform distribution, we often use $x = -\frac{1}{\theta} \log(u)$ instead

- ▶ Normal distribution: $f(x) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{x^2}{2})$. **Box-Muller Transform**

$$X = \sqrt{-2 \log U_1} \cos 2\pi U_2$$

$$Y = \sqrt{-2 \log U_1} \sin 2\pi U_2$$

where $U_1 \sim \text{Uniform}(0, 1)$, $U_2 \sim \text{Uniform}(0, 1)$



- ▶ Assume $Z = (X, Y)$ follows the standard bivariate normal distribution. Consider the following transform

$$X = R \cos \Theta, \quad Y = R \sin \Theta$$

- ▶ From symmetry, clearly Θ follows the uniform distribution on the interval $(0, 2\pi)$ and is independent of R
- ▶ What distribution does R follow? Let's take a look at its CDF

$$\begin{aligned} p(R \leq r) &= p(X^2 + Y^2 \leq r^2) \\ &= \frac{1}{2\pi} \int_0^r t \exp\left(-\frac{t^2}{2}\right) dt \int_0^{2\pi} d\theta = 1 - \exp\left(-\frac{r^2}{2}\right) \end{aligned}$$

Therefore, using the inverse CDF rule, $R = \sqrt{-2 \log U_1}$

- ▶ If it is difficult or computationally intensive to sample directly from $f(x)$ (as described above), we need to use other strategies
- ▶ Although it is difficult to sample from $f(x)$, suppose that we can evaluate the density at any given point up to a constant $f(x) = f^*(x)/Z$, where Z could be unknown (remember that this makes Bayesian inference convenient since we usually know the posterior distribution only up to a constant)
- ▶ Furthermore, assume that we can easily sample from another distribution with the density $g(x) = g^*(x)/Q$, where Q is also a constant

- ▶ Now we choose the constants c such that $cg^*(x)$ becomes the envelope (blanket) function for $f^*(x)$:

$$cg^*(x) \geq f^*(x), \quad \forall x$$

- ▶ Then, we can use a strategy known as *rejection sampling* in order to sample from $f(x)$ indirectly
- ▶ The rejection sampling method works as follows
 1. draw a sample x from $g(x)$
 2. generate $u \sim \text{Uniform}(0, 1)$
 3. if $u \leq \frac{f^*(x)}{cg^*(x)}$ we accept x as the new sample, otherwise, reject x (discard it)
 4. return to step 1

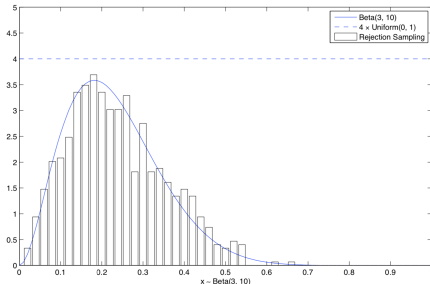


Rejection sampling generates samples from the target density, no approximation involved

$$\begin{aligned} p(X^R \leq y) &= p(X^g \leq y | U \leq \frac{f^*(X^g)}{cg^*(X^g)}) \\ &= p(X^g \leq y, U \leq \frac{f^*(X^g)}{cg^*(X^g)}) / p(U \leq \frac{f^*(X^g)}{cg^*(X^g)}) \\ &= \frac{\int_{-\infty}^y \int_0^{\frac{f^*(z)}{cg^*(z)}} dug(z) dz}{\int_{-\infty}^{\infty} \int_0^{\frac{f^*(z)}{cg^*(z)}} dug(z) dz} \\ &= \int_{-\infty}^y f(z) dz \end{aligned}$$



- ▶ Assume that it is difficult to sample from the $\text{Beta}(3, 10)$ distribution (this is not the case of course)
- ▶ We use the $\text{Uniform}(0, 1)$ distribution with $g(x) = 1, \forall x \in [0, 1]$, which has the envelop property: $4g(x) > f(x), \forall x \in [0, 1]$. The following graph shows the result after 3000 iterations

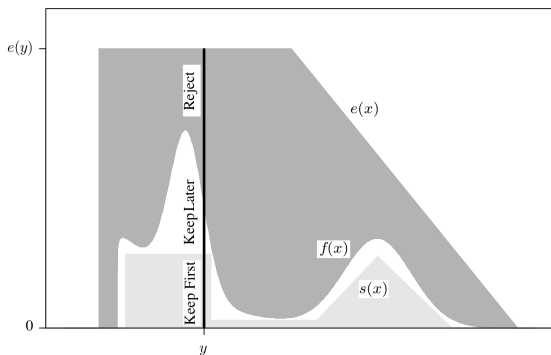


Rejection sampling becomes challenging as the dimension of x increases. A good rejection sampling algorithm must have three properties

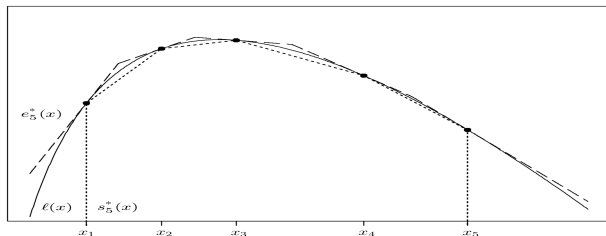
- ▶ It should be easy to construct envelopes that exceed the target everywhere
- ▶ The envelop distributions should be easy to sample from
- ▶ It should have a low rejection rate

- ▶ When evaluating f^* is computationally expensive, we can improve the simulation speed of rejection sampling via *squeezed rejection sampling*
- ▶ Squeezed rejection sampling reduces the evaluation of f via a nonnegative squeezing function s that does not exceed f^* anywhere on the support of f : $s(x) \leq f^*(x), \forall x$
- ▶ The algorithm proceeds as follows:
 1. draw a sample x from $g(x)$
 2. generate $u \sim \text{Uniform}(0, 1)$
 3. if $u \leq \frac{s(x)}{cg^*(x)}$, we accept x as the new sample, return to step 1
 4. otherwise, determine whether $u \leq \frac{f^*(x)}{cg^*(x)}$. If this inequality holds, we accept x as the new sample, otherwise, we reject it.
 5. return to step 1



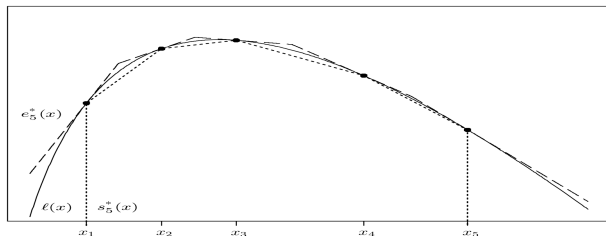


Remark: The proportion of iterations in which evaluation of f is avoided is $\int s(x)dx / \int e(x)dx$



- ▶ For a continuous, differentiable, log-concave density on a connected region of support, we can adapt the envelope construction (Gilks and Wild, 1992)
- ▶ Let $T = \{x_1, \dots, x_k\}$ be the set of k starting points.
- ▶ We first sample x^* from the piecewise linear upper envelope $e(x)$, formed by the tangents to the log-likelihood ℓ at each point in T_k .





- ▶ To sample from the upper envelop, we need to transform from log space by exponentiating and using properties of the exponential distribution
- ▶ We then either accept or reject x^* as in squeeze rejection sampling, with $s(x)$ being the piecewise linear lower bound formed from the chords between adjacent points in T
- ▶ Add x^* to T whenever the squeezing test fails.



- ▶ P. J. Davis and P. Rabinowitz. *Methods of Numerical Integration*. Academic, New York, 1984.
- ▶ W. R. Gilks and P. Wild. Adaptive rejection sampling for Gibbs sampling. *Applied Statistics*, 41:337–348, 1992.