

CS 70 - Foundations Of Applied Computer Science

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Reading Assignment 6

CS 70 - Chapter 11 (Numerical Integration)

Deterministic Quadrature: You may recall that integrals can be numerically evaluated using quadrature methods (such as a Riemann sum, or the trapezoid or Simpson rules). These can typically be expressed as the weighted sum

$$F = \int_a^b f(x) dx \approx \sum_{i=1}^n w_i f(x_i)$$

where the different quadrature rules dictate the placement of the points x_1, \dots, x_n and the weights w_i for each point.

Monte Carlo Integration: The basic idea of Monte Carlo integration is very simple: it transforms the problem of integration into one of estimating an expected value. The trick is to first construct a random variable whose expected value is equal to our integral of interest. Monte Carlo then estimates this expected value by averaging random realizations of the variable, which in turn approximates the integral.

Suppose that we want to integrate the (potentially multidimensional) function $f(x)$ over some domain D

$$F = \int_D f(x) dx$$

We define the random variable

$$\hat{F} = \frac{f(X)}{p(X)}$$

as the ratio between the integrand evaluated at a random point X and the probability density $p(X)$ of choosing the point X .

The Monte Carlo estimator approximates the expression by averaging many independent samples of \hat{F} :

$$F \approx \hat{F}_n = \frac{1}{N} \sum_{i=1}^N \hat{F}_i = \frac{1}{N} \sum_{i=1}^N \frac{f(x_i)}{p_X(x_i)}$$

where the x_i are independent and individually distributed samples drawn from the PDF $p_X(x_i)$.

The Law of Large Numbers: The LLN states that the average of many independent realizations of a random variable will converge to the expected value of the random variable with virtual certainty.

$$\hat{F}_N \rightarrow F \text{ as } N \rightarrow \infty$$

Variance, Standard Deviation, & Convergence Rate: We can quantify how quickly we approach the correct answer by calculating the variance (squared error) and standard deviation (error):

$$\begin{aligned}\mathbb{V}[\hat{F}_N] &= \frac{1}{N} \mathbb{V}[\hat{F}] \\ \sigma[\hat{F}_N] &= \frac{1}{\sqrt{N}} \sigma[\hat{F}]\end{aligned}$$

The Central Limit Theorem (CLT): The CLT tells us that the sum (or average) of N iid random variables will converge to a normal distribution as $N \rightarrow \infty$, even if the original variables are not themselves normally distributed. Hence, \hat{F}_N will approach a normal distribution, with mean F and variance $\mathbb{V}[\hat{F}]/N$, as N increases. We can use this property to compute confidence intervals around our estimate \hat{F}_N .

Transforming & Sampling Random Variables: In order to evaluate the Monte Carlo estimator, we need to be able to draw samples X from some desired distribution p_X .

Transforming Random Variables (Univariate Case): Passing a random variable $X \sim p_X(x)$ through an invertible function $T: \mathbb{R} \rightarrow \mathbb{R}$ produces another random variable Y . We consider two approaches for computing the PDF $p_Y(y)$ of Y .

CDF Approach Find the CDF.

$$P_Y(y) = \mathbb{P}(Y \leq y)$$

Differentiate the CDF to obtain the PDF.

$$p_Y(y) = \frac{d}{dy} P_Y(y)$$

Change-Of-Variables Approach Alternatively, we can use the change-of-variables approach.

$$p_Y(y) = p_X(T(x)) = \frac{p_X(x)}{|T'(x)|} = \frac{p_X(T^{-1}(y))}{|T'(T^{-1}(y))|'}$$

where $|T'(x)|$ is the absolute value of the derivative $\frac{d}{dx}T(x)$ of the transformation T .

Sampling Random Variables (The Inversion Method): The inverse of the above process is called the inversion method (for univariate random variables). Typically we start with a uniform random variable $Y \in [0, 1)$, and want to determine a function $T: \mathbb{R} \rightarrow \mathbb{R}$ so that $X = T(Y)$ has some desired distribution $X \sim p_X(x)$.

We can accomplish this with the following 3-step procedure.

Compute the CDF of the desired distribution.

$$P_X(x) = \int_{-\infty}^x p_X(x') dx'$$

Compute the inverse of the CDF.

$$P_X^{-1}(y) \text{ by setting } T(Y) = P_X^{-1}(Y)$$

Pass Y through the inverse CDF.

$$X = P_X^{-1}(Y)$$

now has the desired distribution.

Multivariate: Transforming and sampling random variables for the multivariate case is appropriately covered in the provided notes.