MS-C1650 Numeerinen analyysi, Exercise 3, Guidelines

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Problem 1

See Lecture notes, Example 6.1.4.

Idea of Monte Carlo: We have a random variable, whose mean should be the quantity we try to compute (the area of an ellipse), and standard deviation measures the reliability of our simulations. These quantities are explored by sampling (using a computer), rather than using pen-and-paper.

This model problem: We know the true values, but let's pretend that we don't. Use Monte Carlo to estimate the expectation and standard deviance.

a-c) A computer is recommended

d) Denote the ellipse by A, and the rectangle by Ω. Randomly generated points inside the rectangle are denoted by (x_i, y_i). The random variable X_i is defined by

$$X_i = \begin{cases} 1 & \text{if } (x_i, y_i) \in A, \\ 0 & \text{otherwise.} \end{cases}$$

The expectation value (i.e., the percentage of random points inside the ellipse) is now estimated by a computer simulation,

$$\mu := \mathrm{E}[X_i] \approx ...$$

The variance (= standard deviation σ squared) of a random variable is defined by

$$\begin{aligned} \sigma^2 = \mathrm{Var}(X_i) &:= \mathrm{E}[(X_i - \mu)^2] = \mathrm{E}[X_i^2 - 2\mu \mathrm{E}[X_i] + \mu^2] \\ &= \mathrm{E}[X_i^2] - 2\mu \mathrm{E}[X_i] + \mu^2 = \mathrm{E}[X_i^2] - 2\mu^2 + \mu^2 \\ &= \mathrm{E}[X_i^2] - \mu^2. \end{aligned}$$

In this case,

$$X_i^2 = ...$$

e) Central Limit Theorem: "Quite often, the average of N independent random variables with the mean μ, standard deviation σ, tends towards a Gaussian distribution with the mean μ and std σ, as N increases" (see Wikipedia or some book for proper definitions). In this case, the average is a random variable

$$A_N := \frac{1}{N} \sum_{i=1}^{N} X_i,$$

with

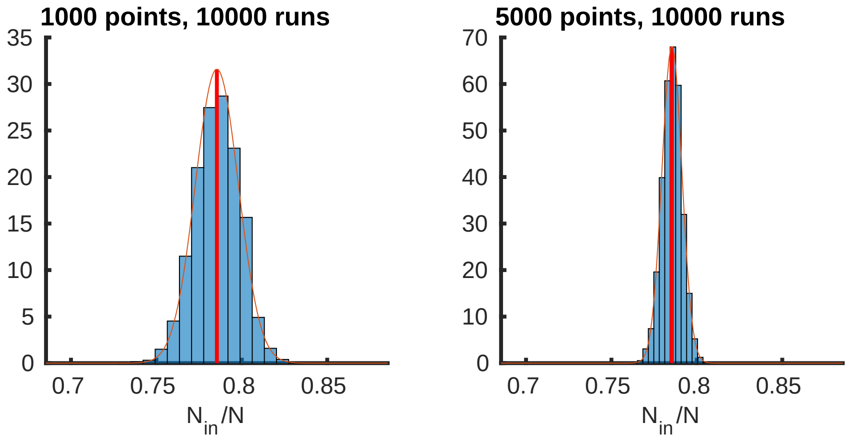
$$\mathrm{E}[A_N] = \mu,$$

and

$$\mathrm{Var}[A_N] = \frac{1}{N^2}\sum_{i=1}^{N} \mathrm{Var}[X_i] = \frac{\sigma^2}{N}.$$

After running N simulations, σ can be estimated by computing...

My test runs with $N = 1000$ and $N = 5000$ points, each of them repeated 10000 times to plot something Gaussian-like. Red bar = true value, histogram = frequency of each simulation, curve = Gaussian with true μ, estimated σ:



The width of the distribution decreases as N increases, as it should be.

f) The exact formula for the area of an ellipse is ...

Problem 2

a) We sample the function at the midpoint of each interval and multiply by the width of the interval, so the integral estimation can be illustrated by...

b) Apply the midpoint rule for $f(x) = cx + d$, where c, d can be any real numbers, and find out that

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = hf(x_{i-1/2}).$$

c) First, consider only a single interval, and try to figure out why

$$\left| \int_{x_{i-1}}^{x_i} f(x)\,dx - hf(x_{i-1/2}) \right| \leq Ch^3.$$

(As explained in the exercise sheet: insert the 1st order Taylor polynomial evaluated at the midpoint + the error term into the integral, and see what happens). Then, the number of intervals n is related to the interval length h as ... so you get the result.

Exercise 3

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In other words, find the weights A_0, A_1 and the sample points x_0, x_1 such that

$$\int_{-1}^{3}(x+1)f(x)\,dx = A_0 f(x_0) + A_1 f(x_1)$$

holds exactly for all functions of form $f(x) = \sum_{i=0}^{3} c_i x^i$.

Method 1: Brute force (Lecture notes 6.3) leads to a nonlinear system of four equations, four unknowns. Is it solvable/how to solve it? But a more elegant method is

Method 2: Denote

$$\langle p, q\rangle_w := \int_a^b p(x)q(x)w(x)\,dx.$$

The polynomials p, q are said to be w-orthogonal, if $\langle p, q\rangle_w = 0$.

Theorem 1 (6.3.4 from the Lecture notes) *Let q be a (nontrivial) polynomial of degree $n+1$ such that*

$$\langle q, x^k\rangle_w = 0 \ \ \textit{for} \ \ k = 0, 1, ..., n. \tag{1}$$

Let $x_0, ..., x_n$ be the roots of q. Then the quadrature rule

$$\int_a^b f(x)w(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

is exact when $f(x)$ is a polynomial of order up to $2n+1$.

Now, we have weight $w = x+1$ and interval $(a, b) = (-1, 3)$, two quadrature points so $n = 1$. The first problem: find the polynomial q that fulfills (1). The space $P_n(a, b)$ denotes order n polynomials in the interval (a, b), and it is a vector space of dimension $n+1$. The bilinear form $\langle\cdot,\cdot\rangle_w$ given above defines an inner product in that space, and you can do "linear algebra".

Orthogonal polynomial 1. We can assume q is monic (leading coefficient is 1), so $q(x) = c_0 + c_1 x + x^2$. Then the equation (1) becomes a linear system

$$\begin{aligned} c_0\langle 1, 1\rangle_w + c_1\langle x, 1\rangle_w &= -\langle x^2, 1\rangle_w \\ c_0\langle 1, x\rangle_w + c_1\langle x, x\rangle_w &= -\langle x^2, x\rangle_w, \end{aligned}$$

from where you can solve c_0, c_1 (warning: numerically bad when the polynomial order is large, Google for Hilbert matrix).

Orthogonal polynomial 2. Use Gram-Schmidt. Construct a w-orthogonal basis $\{v_0, v_1, v_2\}$ for the space $P_2(-1, 3)$, where $P_n(a, b)$ denotes order n polynomials in the interval (a, b), and $v_i \in P_i(-1, 3)$. This can be done by Gram-Schmidt, starting from the monomial basis $\{1, x, x^2\}$:

$$\begin{aligned} v_0 &= 1 \\ v_1 &= x - \frac{\langle x, v_0\rangle_w}{\langle v_0, v_0\rangle_w} v_0 \\ v_2 &= x^2 - \frac{\langle x^2, v_0\rangle_w}{\langle v_0, v_0\rangle_w} v_0 - \frac{\langle x^2, v_1\rangle_w}{\langle v_1, v_1\rangle_w} v_1 \end{aligned}$$

Now, why $q := v_2$ is a polynomial satisfying (1)?

Do a reality check with your polynomial: verify $\langle q, 1\rangle_w = 0$ and $\langle q, x\rangle_w = 0$. The quadrature points x_0, x_1 are the zeros of q. (By some theorem, the quadrature points have to be inside (a, b) [??]). Finally, you can figure out the weights A_0, A_1 by one way or another.

Exercise 4

Brute force: Insert $f(x) = a_0$, $f(x) = a_0 + a_1 x$, $f(x) = a_0 + a_1 x + a_2 x^2$ etc and see when the quadrature rule fails to be exact for arbitrary a_n.

More clever: ?

MATLAB

a) Compute the Taylor polynomial coefficients at $x_0 = 0$ by one way or another. Plot the obtained Taylor polynomials of different orders, along with the original function $f(x) = e^{\sin(\pi x)}$. Integrate the Taylor polynomial(s) over $[-1, 1]$. The result: probably bad.

b) The n-point Gauss-Legendre quadrature rule integrates polynomial up to order $2n - 1$ exactly. Thus, use the Taylor theorem

$$f(x) = f(0) + f'(0)x + \frac{1}{2!}f''(0)x^2 + ... + \frac{1}{(2n-1)!}f^{2n-1}(0) + R_{2n}(x),$$

with a suitable formula for the remainder term. Estimate the error $\int_{-1}^{1} R_{2n}(x)\,dx$ somehow. You will probably get a very pessimistic estimate (i.e., the actual error is muuuuch smaller than the estimate).

Morale of the story (a-b): a Taylor polynomial $P_n(x) \approx e^{\sin(\pi x)}$ is not a good approximation in the interval $[-1, 1]$. (But the Gauss quadrature rule should be ok).

The next question: How do you get a sensible error estimate? Ask the lecturer, if you really want to know.

c) Compute the "exact" value $I_{\text{true}} = \int_{-1}^{1} f(x)\,dx$ up to very many digits (use premade libraries or whatever comes into your mind), and compare the results $I_n \approx \int_{-1}^{1} f(x)\,dx$ obtained by an n-point quadrature rule with I_{true}. Plot the error (maybe using a log-plot or something similar, as in the 1st Exercise round).

CHALLENGE

Haven't tried. Only if someone asks...