C1 MA913 Scientific Computing 2015/2016

Assignment 4

Solve at least two of the following three exercises.

Monte Carlo integration. We are interested in calculating the following integral

$$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x}$$

for some given function f. We try different cases, which mainly differ by the degree of regularity of the function f. For at least two of the functions listed below:

- Write a Monte Carlo estimator to numerically estimate the integral of f. It is preferable for statistical purposes (but more memory intensive), for a given dimension N and number of samples M, to write a routine that generates MN random samples on $[0,1]$ (or equivalently M random points in the hyper-cube $[0,1]^N$) all together, instead of sampling one single number at a time. This allows us to have distinct and independent samples when we change N or M and study the convergence rate.
- Estimate the error using the Central Limit Theorem. Plot the exact error and error estimates versus the number of samples used. Estimate the convergence rate. Do your computations at least for $N = 2$ and $N = 10$.
- Discuss the results with respect to the regularity of the functions and the dimension of the problem.
- *Optional:* compare the results with deterministic quadrature rules (e.g. mid-point).

List of functions:

(1) Oscillatory: $f(\mathbf{x}) = \cos\left(2\pi w_1 + \sum_{n=1}^N c_n x_n\right)$, with $c_n = 9/N$, $w_1 = \frac{1}{2}$.
Exact solution:

$$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \Re\left(e^{i2\pi w_1} \prod_{n=1}^N \frac{1}{ic_n}(e^{ic_n} - 1)\right)$$

(here i denotes the imaginary unit and $\Re(z)$ the real part of $z \in \mathbb{C}$)

(2) Product peak: $f(\mathbf{x}) = \prod_{n=1}^N \left(c_n^{-2} + (x_n - w_n)^2\right)^{-1}$, with $c_n = 7.25/N$ and $w_n = \frac{1}{2}$.
Exact solution:

$$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \prod_{n=1}^N c_n\left(\arctan(c_n(1 - w_n)) + \arctan(c_n w_n)\right)$$

(3) Gaussian: $f(\mathbf{x}) = \exp\left(-\sum_{n=1}^N c_n^2(x_n - w_n)^2\right)$, with $c_n = 7.03/N$ and $w_n = \frac{1}{2}$.
Exact solution:

$$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \prod_{n=1}^N \frac{\sqrt{\pi}}{2c_n}\left(\operatorname{erf}(c_n(1 - w_n)) + \operatorname{erf}(c_n w_n)\right)$$

(4) Continuous: $f(\mathbf{x}) = \exp\left(-\sum_{n=1}^N c_n|x_n - w_n|\right)$,with $c_n = 2.04/N$ and $w_i = \frac{1}{2}$.
Exact solution:

$$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \prod_{n=1}^N \frac{1}{c_n}\left(2 - e^{-c_n w_n} - e^{-c_n(1-w_n)}\right)$$

(5) Discontinuous:

$$f(\mathbf{x}) = \begin{cases} 0 & \text{if } x_1 > w_1 \text{ or } x_2 > w_2 \\ \exp\left(\sum_{n=1}^N c_n x_n\right) & \text{otherwise,} \end{cases}$$

with $c_i = 4.3/N$, $w_1 = \frac{\pi}{4}$ and $w_2 = \frac{\pi}{5}$.
Exact solution:

$$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \frac{1}{\prod_{n=1}^{N} c_n}(e^{c_1 w_1} - 1)(e^{c_2 w_2} - 1)\prod_{n=3}^{N}(e^{c_n} - 1)$$

(6) Simplex:

$$f(\mathbf{x}) = \begin{cases} 1 & \text{if } \sum_n x_n \le 1 \\ 0 & \text{otherwise.} \end{cases}$$

Exact solution:

$$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \frac{1}{N!}.$$

ODEs with uncertain parameters. Consider the problem 1b in assignment 3 when parameters are not exactly know and therefore modeled as random variable. Let the two parameters, λ and μ, be independent random variables, distributed according to a lognormal law, i.e.,

$$\lambda = \exp\left(\mathcal{N}(\eta, \sigma^2)\right)$$

where $\mathcal{N}$ indicates the normal (Gaussian) distribution with mean η and variance σ^2. If we assume λ to have mean $E[\lambda] = \lambda_0$ (equal to the value in assignment 3) and a certain variance $V[\lambda] = \lambda_{STD}^2$, the normal distribution should have

$$\eta = \ln\left(\frac{\lambda_0}{\sqrt{1 + \frac{\lambda_{STD}^2}{\lambda_0^2}}}\right), \qquad \sigma = \sqrt{\ln\left(1 + \frac{\lambda_{STD}^2}{\lambda_0^2}\right)}$$

and similarly for parameter μ (initially you could just consider one parameter constant and the other random and, if time allows, consider both to be random).
Consider μ and λ with their mean equal to the values in assignment 3 and variances of your choice, implement a random sampling from their distribution (you can use this example code that samples from normal distributions), fix a time T of your choice, for each sample of λ and μ solve the ODE with the code you developed for assignment 3 (remember that λ and μ can be sampled independently), and compute a Monte Carlo approximation for

$$E[u(T)],\ V[u(T)],\ E[v(T)],\ V[v(T)]$$

where E is the expected value and V is the variance.

- Run the estimation for different number of samples N (e.g., 2^i, $i = 3, \ldots, 12$) and check the convergence of the sample mean to the exact or reference solution[1].
- From these results (and the ones in assignment 3), try to understand and comment on the role and relative magnitude of the discretisation errors in the Monte Carlo integration and in the ODE solver.
- Plot the results of the ODE integration in time for different random realizations to show the variability in the dynamics, or plot the histogram for $v(T)$.
- *Suggestion:* try to understand the computing time (number of Monte Carlo samples times ODE runs) required to compute a reasonably accurate mean (e.g., 1%) for given T and variances, and then choose them appropriately to have a code that runs in reasonable time.
- *Optional:* repeat a similar exercise for problem 2b (the Lorentz attractor), considering uniform distributions for the parameters, centered around the values given in assignment 3.

[1] The analytical solution given in assignment 3, computed at a time T, appropriately chosen, can be analytically integrated against the lognormal distributions, and the mean and variance of the solution can be computed exactly. Alternatively a reference solution can be computed integrating numerically the analytical solution at time T with a large number of Monte Carlo samples or high-order quadrature rule.

- *Optional:* repeat the same integration (over the probability distribution of the parameters) with a deterministic quadrature rule (e.g., change variable in the integral to transform the integral against the lognormal PDF to a normal PDF and then use Gauss-Hermite quadrature points weights) and compare results. Can you comment on the regularity of the integrand function and the requirement of the Monte Carlo method vs deterministic methods?

Advection-Diffusion equation. Consider the linear advection diffusion problem described in the lectures (see Section 12.5 of the book "Numerical Mathematics" by Quarteroni, Sacco, Saleri, eq. 12.70), i.e.

$$-\alpha u'' + \beta u' = 0, \qquad u(0) = 0,\ u(L) = 1$$

in the domain $\Omega = [0, L]$. Consider at least 3 different values of the parameters such that the Peclet number $Pe = \frac{|\beta| L}{2\alpha}$ is first zero, then around unity, then rather large.
Discretise the equation by at least one of the following methods:

- Linear Finite Elements (Eq. 12.75)
- Finite differences (Eq. 12.77 or 12.78 or any other finite difference scheme of your choice)
- Spectral method (Eq. 12.68 computing the integral analytically using a family of orthogonal polynomials of your choice)
- Pseudo-spectral method (Eq. 12.68 computing the integral with a Gauss-Lobatto quadrature; or, equivalently, assuming as the test function space the span of delta functions centred in the Gauss-Lobatto nodes; or directly using the pseudo-spectral differentiation matrix 10.73 as described in Section 12.3)
- Finite Volume method with central scheme (e.g., Galerkin method with piecewise linear continuous trial functions and piecewise constant discontinuous test functions. To obtain the standard finite volume formulation, the problem should be formulated using, as variables, the integral of u against the test functions, i.e. the mean value in each cell, instead of the coefficients with respect to the basis of the trial function space.)

Plot the solution for a few different mesh sizes (or polynomial orders) and the error with respect to the analytical solution

$$u(x) = \frac{\exp(\frac{\beta x}{\alpha}) - 1}{(\exp(\frac{\beta L}{\alpha}) - 1)}$$

using a norm of your choice (depending on the method it might be easier to compute the L^2 or a discrete norm). Try to understand the order of convergence of the method and a theoretical result justifying it.

Submission. For the submission follow the same instructions provided with assignment 1. Given the complexity of this assignment, the reproducibility requirement will be considered only for extra points and not strictly required

Deadline: Friday 8th January 2016 6:00 pm