

Homework #1 is due the beginning of class on Thursday, April 28, although you may submit an electronic version before then. Each person should turn in his or her own write-up. No late homeworks will be accepted.

Problem 1. Concepts

- A. Let Y be a Bernoulli random variable taking values in $\{0, 1\}$ with success parameter p . Suppose we draw n independent samples of Y ; let T be the number of successes in n samples. Then T is a binomial random variable with distribution

$$\mathbb{P}(T = t) = \binom{n}{t} p^t (1 - p)^{n-t}.$$

Given t successes, an exact 99% confidence interval $p_L \leq p \leq p_U$ can be found by solving

$$0.005 = \sum_{i=t}^n \binom{n}{i} p_L^i (1 - p_L)^{n-i}$$
$$0.005 = \sum_{i=0}^t \binom{n}{i} p_U^i (1 - p_U)^{n-i}.$$

Suppose that $n = 10,000$ and $t = 17$. Compute p_L and p_U .

- B. The procedure for stably computing the variance estimate s^2 on samples y_i with one pass through the data is as follows. Let $S_n = \sum_{i=1}^n (y_i - \mu_n)^2$. Starting with $\mu_1 = y_1$ and $S_1 = 0$, make the updates for $i = 2, \dots, n$:

$$\delta_i = y_i - \mu_{i-1}$$
$$\mu_i = \mu_{i-1} + \frac{1}{i} \delta_i$$
$$S_i = S_{i-1} + \frac{i-1}{i} \delta_i^2$$

Then $s^2 = S_n/(n-1)$. Prove that this update procedure produces the correct variance estimate.

- C. Li & Xiu (JCP, 2010) propose a method to estimate a probability of failure using a *surrogate model*. Loosely speaking, the surrogate approximates the output of an expensive simulation at a given input parameter with much less computational effort. Derive confidence bounds for their estimate of the failure probability. If necessary, assume you know the error in the surrogate model. Is this estimate unbiased?

Problem 2. Programming

Download the zip file `hw1_code.zip` from the website. This contains a MATLAB script for computing the output of a complex simulation of great national interest (not really). You can run this simulation from within MATLAB by providing a grid resolution parameter m and model parameter s using the syntax

$$\mathbf{x} = \text{complex_solver}(s,m);$$

The parameter s can take values in the interval $[-1, 1]$ with a uniform density. The output x is a vector of length $n - 1$. Let $y(s) = \max_i x_i(s)$, where x_i is the i th component of the output. It is of utmost importance that you determine

$$p^* = \mathbb{P}(y \geq 0.2).$$

Complete the following exercises.

- A. Use simple Monte Carlo to compute 99% confidence bounds for p^* with grid resolution parameter $m = 1001$. Plot the relative change in these bounds for $n = 10, 100, 1000, 10000$ samples.
- B. Suppose I tell you that $y(s)$ is a monotonic function of s . First, verify this. Second, devise and implement an importance sampling strategy to compute 99% confidence bounds on p^* that takes advantage of this information.
- C. Use Li & Xiu's method to estimate p^* and report your results and experiences. Use your favorite non-intrusive surrogate model with the given complex solver. If you do not yet have a favorite surrogate model, you may either use the polynomial approximation procedure described in the paper or the same complex solver code with grid resolution $m = 101$. (If you're feeling ambitious, try both!) How much did this improve the simulation time? How accurate are its results? Can you apply the confidence bounds you derived above?

Problem 3. Reading

Read the following papers.

- A. Jing Li and Dongbin Xiu. *Evaluation of failure probability via surrogate models*. Journal of Computational Physics, 2010.
- B. Qiqi Wang, Karthik Duraisamy, Juan Jose Alonso, and Gianluca Iaccarino. *Risk Assessment of Scramjet Unstart Using Adjoint-Based Sampling Methods*. AIAA 2010-2921.
- C. Christopher J. Roy and William L. Oberkampf. *A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing*. Computer Methods in Applied Mechanics and Engineering, 2011.

Write a one-page critical response to one of the papers. You should summarize the work in a paragraph and attempt to answer questions such as: How might you apply these ideas to your own research? What are the primary advantages and disadvantages of the methods? How might the methods or concepts be improved?