## CZ3272 Monte Carlo and Molecular Dynamics

## Tutorial 1 (for week 2-3, starting 21 August 06)

A good book on probability, although somewhat advanced, is "Statistical Inference",  $2^{nd}$  edition, by G Casella and R L Berger. Work on these problems while I'm away during week 3. Required to submit by week 4 (5 Sep 06).

1. Consider a toss experiment of two coins, say, a dollar and a 50-cent coin. (a) What is the sample space S? Enumerate the elements in S. (b) What is the probability of each possible outcome, assuming fair coin tosses? (c) Verify that the equation  $P(A \cup B) = P(A) + P(B) - P(A \cap B)$  is true when A represents the event dollar gets a head, and B represents the event 50-cent gets a head. (d) Since A and B are subsets of S, enumerate the elements in A and B.

**2**. Approximately one-third of all human twins are identical (one-egg) and two-thirds are fraternal (two-egg) twins. Identical twins are necessarily the same sex, with male and female being equally likely. Among fraternal twins, approximately one-fourth are both female, one-fourth are both male, and half are one male and one female. Finally, among all Singapore births, approximately 1 in 90 is a twin birth. Define the following events:

A = { a Singapore birth results in twin females}
B = { a Singapore birth results in identical twins }
C = { a Singapore birth results in twins }
(a) State, in words, the events A ∩ B ∩ C.

(b) Find  $P(A \cap B \cap C)$ .

**3**. Prove or show it is plausible each of the following statements (assuming that any conditioning event has positive probability).

(a) If P(B) = 1, then P(A|B) = P(A) for any A.

(b)  $A \subset B$ , then P(B|A) = 1, and P(A|B) = P(A)/P(B).

(c) If A and B are mutually exclusive, then  $P(A|A \cup B) = P(A)/(P(A) + P(B)).$ 

(d)  $P(A \cap B \cap C) = P(A|B \cap C) P(B|C) P(C)$ .

**4**. In the Buffon needle problem, prove the probability of the needle intersecting the equally spaced line is  $P = 2L/(\pi d)$ , where L is the length of the needle, and d is strip spacing, and L < d.

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## Lab 1 (for week 3-4, starting 28 Aug 06)

Submitting by end of week 4 (8 Sep 06)

- **1**. This lab is about random number generator.
  - (a) Implement the Hayes 64-bit linear congruential random number generator in C (as a function), that is, a = 6364136223846793005, c = 1,  $m = 2^{64}$ , with the recursion relation  $x_{n+1}=(a x_n+c) \mod m$ . The return value should be a normalized double precision number in the interval [0, 1). Use long long int data type for the calculation. [We'll need this program for the later labs].
  - (b) To verify that your program works as intended, check that the first few numbers  $x_n$  are (assuming  $x_0=1$ ):
    - n x<sub>n</sub>
    - 0 1
    - 1 6364136223846793006
    - 2 13885033948157127959
    - 3 14678909342070756876
    - 4 14340359694176818205
    - 5 ...
  - (c) Perform a chi-square test for the uniform-ness of the distribution. Conclude from this test if the random number is indeed uniformly distributed. Read page 42-47, "The Art of Computer Programming" Vol 2 Seminumerical Algorithms, 3<sup>rd</sup> edition, by D E Knuth about chi-square test.
  - (d) Finally, timing the speed of your implementation of the random number generator. Report in units of microsecond  $(10^{-6} \text{ second})$  per function call.