Simulation for a pair of biallelic Loci in LD

The purpose of this note is to give an introduction that how to simulate a pair of loci, which is in gametic disequilibrium. s the commonly used gametic disequilibrium parameter, D, has its upper bound and lower bound upon to the allele frequencies, it seems to be easier to simulate a pair of loci given D', the relative gematic disequilibrium as defined by Lewontin, the value of which is between -1 to 1.

Let the allele frequency of locus A is of f_A for allele A and of $1-f_A$ for a, and of locus B is of f_B for B and of $1-f_B$ for b. The frequencies of the four haplotypes of these two loci are f_{AB} (haplotype AB), f_{Ab} (haplotype Ab), f_{aB} (haplotype aB), and f_{ab} (haplotype ab). The Lewontin's measure [Lewontin 1964] of linkage disequilibrium, which is a quantity between -1 and 1, can be specified first for a pair of loci of question

$$D' = \begin{cases} \dfrac{D}{\min\left(f_A(1-f_B), f_B(1-f_A)\right)}, D > 0 \\ \dfrac{D}{\min\left(f_A f_B, (1-f_A)(1-f_B)\right)}, D < 0 \end{cases}$$

in which $D = f_{AB} - f_A f_B = f_{AB} f_{ab} - f_{Ab} f_{aB}$[Devlin and Risch 1995]. Regardless of the sign of D, the denominator in the expression of D' is denoted as ψ, and $D = D' \times \psi$.

		Locus A		
		A (1)	a (0)	
Locus B	B (1)	AB $f_A f_B + D$	aB $(1-f_A)f_B - D$	f_B
	b (0)	Ab $f_A(1-f_B) - D$	ab $(1-f_A)(1-f_B) + D$	$1-f_B$
		f_A	$1-f_A$	

In simulation, under random mating, the conditional probability of generating the second locus could be expressed as (t is generation)

$$P(L_B = l_B | L_A = l_A) = \frac{f_{l_B} f_{l_A} + (-1)^{|l_B - l_A|} D^t}{f_{l_A}}$$

and l_X indicates the allele. $l_A = 1$, if the allele is A, and 0 for a. Similar for l_B.

$$P(L_B = 1 | L_A = 1) = \frac{P(L_B = 1, L_A = 1)}{f_A} = \frac{f_A f_B + D^t}{f_A}$$

$$P(L_B = 0 | L_A = 1) = \frac{P(L_B = 0, L_A = 1)}{f_A} = \frac{f_A(1-f_B) - D^t}{f_A}$$

$$P(L_B = 1 | L_A = 0) = \frac{P(L_B = 1, L_A = 0)}{1-f_A} = \frac{(1-f_A)f_B - D^t}{1-f_A}$$

$$P(L_B = 0 | L_A = 0) = \frac{P(L_B = 0, L_A = 0)}{1-f_A} = \frac{(1-f_A)(1-f_B) + D^t}{1-f_A}$$