

To the Graduate Council:

I am submitting herewith a thesis written by Mahendra Duwal Shrestha entitled “Analysis and Simulation Of A Simple Evolutionary System.” I have examined the final paper copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Computer Science.

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Michael D. Vose, Major Professor

We have read this thesis  
and recommend its acceptance:

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Committee Member 1

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Committee Member 2

Accepted for the Council:

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Dixie Thompson

Vice Provost and Dean of the Graduate School

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(Original signatures are on file with official student records.)

# Analysis and Simulation Of A Simple Evolutionary System

A Thesis Presented for

The Master of Science

Degree

The University of Tennessee, Knoxville

Mahendra Duwal Shrestha

August 2016

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*dedication...*

# Acknowledgements

I would like to thank...

*Some quotation...*

# Abstract

Abstract text goes here...



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# Chapter 1

## Introduction

### 1.1 Introduction

### 1.2 Literature

### 1.3 Random Heuristic Search

Vose [Vose \(1999a\)](#) introduced abstract model, a generalized heuristic search method referred to as *Random Heuristic Search (RHS)* which is defined upon the central concept of state and transition between states. An instance of *RHS* can be thought of as an initial collection of elements  $P_0$  chosen from some search space  $\Omega$ , together with a stochastic transition rule  $\tau$ , which from  $P_i$  will produce another collection  $P_{i+1}$ . In other words,  $\tau$  will be iterated to produce a sequence of generations.

The beginning collection  $P_0$  is referred to as the *initial population*. Let  $n$  be the cardinality of  $\Omega$  and  $\mathbf{1}$  denotes column vector of all 1s. The *simplex* is defined to be the set of population descriptors:

$$\Lambda = \langle x_0, \dots, x_{n-1} \rangle : \mathbf{1}^T x = 1, x_j \geq 0$$

An element  $p$  of  $\Lambda$  corresponds to a population according to the rule:

$p_j$  = the proportion in the population of the  $j$ th element of  $\Omega$

The cardinality of each population is a constant  $r$ , called the population size. Given  $r$ , a population descriptor  $p$  unambiguously determines a population.

Given the current population vector  $p$ , the next population vector  $\tau(p)$  cannot be predicted with certainty because  $\tau$  is stochastic and results from  $r$  independent, identically distributed random choices. Let  $\mathcal{G} : \Lambda \rightarrow \Lambda$  be a function that given the current population vector  $p$  produces a new vector whose  $i$ th component is the probability that  $i$ th element of  $\Omega$  is chosen. Thus,  $\mathcal{G}(p)$  is the probability vector that specifies the distribution from which the aggregate of  $r$  choices forms the subsequent generation. Probability that population  $q$  given current population vector  $p$  can be computed as Vose (1999a)

$$r! \prod \frac{(\mathcal{G}(p)_j)^{rq_j}}{(rq_j)!}$$

$$= \exp\left\{-r \sum q_j \ln \frac{q_j}{\mathcal{G}(p)_j} - \sum (\ln \sqrt{2\pi rq_j} + \frac{1}{12rq_j + \theta(rq_j)}) + O(\ln r)\right\}$$

where summation is restricted to indices for which  $q_j > 0$ .

Each random vector in the sequence  $p, \tau(p), \tau^2(p), \dots$  depends only on the value of the preceding one, which is a special situation, and such a sequence forms a Markov chain with transition matrix

$$Q_{p,q} = r! \prod \frac{(\mathcal{G}(p)_j)^{rq_j}}{(rq_j)!}$$

So the conceptualization of RHS can be replaced by Markov chain model abstraction which makes no reference to sampling  $\Omega$ . That is from current population  $p$ , produce  $q = \tau(p)$  with probability  $Q_{p,q}$ . With transition matrix defined for Markov chain model, Vose Vose (1999a) says the expected next generation  $\mathcal{E}(\tau(p))$  is  $\mathcal{G}(p)$  and the expression in transition matrix

$$\sum q_j \ln \frac{q_j}{\mathcal{G}(p)_j}$$

gives the qualitative information regarding probable next generation which is the *discrepancy* of  $q$  with respect to  $\mathcal{G}(p)$ . It is a measure of how far  $q$  is from the expected next population  $\mathcal{G}(p)$ . Discrepancy is nonnegative and is zero only when  $q$  is the expected next population. Hence the factor

$$\exp\{-r \sum q_j \ln \frac{q_j}{\mathcal{G}(p)!}\}$$

in the expression of transition matrix indicates the probability that  $q$  is the next generation decays exponentially, with constant  $r$ , as the discrepancy between  $q$  and the expected next population increases. The expression

$$\sum (\ln \sqrt{2\pi r q_j} + \frac{1}{12r q_j + \theta(r q_j)})$$

measures the *dispersion* of the population vector  $q$  and the factor

$$\exp\{-\sum (\ln \sqrt{2\pi r q_j} + \frac{1}{12r q_j + \theta(r q_j)})\}$$

indicates the probability that  $q$  is the next generation decays exponentially with increasing dispersion.

Vose (1999a) calculated variance of next generation population with respect to expected population as

$$\mathcal{E}(\|\tau(p) - \mathcal{G}(p)\|^2) = (1 - \|\mathcal{G}(p)\|^2)/r$$

and mentioned  $\tau(p)$  converges in probability to  $\mathcal{G}(p)$  as the population size increases. Therefore,  $\tau$  corresponds to  $\mathcal{G}$  in the infinite population case.

## Chapter 2

# Extending A Genetic Algorithm Model To The Diploid Case

This chapter describes a simple Markov model for evolution under the influence of crossing over and mutation; it is a non-overlapping, generational, infinite population model under the assumption of *complete panmixia* (random mating) and no selective pressure. This chapter contributes to the elegance and simplicity of the abstract development and manifests diploid evolution equations can be represented by haploid equations.

A basic syntactic model for haploid and diploid genomes is considered in the beginning and commented on its expressive power. Then the mechanics of how the  $(n + 1)$ th generation is obtained from the  $n$ th generation are defined abstractly in procedural terms, which serves to motivate the equations governing evolution.

Next evolution equations are developed corresponding to the procedural description defining evolution for a population of diploid genomes. Observations concerning the form and symmetry of those equations directly lead to decoupling from the diploid case a haploid model sufficient to determine evolutionary trajectories for the diploid case.

## 2.1 Model

A haploid genome  $g$  is defined syntactically as a length  $\ell$  binary string. A collection of  $h$  chromosomes may be modeled by partitioning  $g$  into  $h$  segments (of arbitrary lengths  $\ell_1, \dots, \ell_h$ ; thus  $\ell = \ell_1 + \dots + \ell_h$ ). Partitioning may be extended to chromosomes so as to interpret each as a collection of genes. If continued to the granularity of pairs of bits, partitioning allows, for example, representing the four possibilities Adenine, Guanine, Cytosine, and Thymine.

A diploid genome  $\alpha = \langle \alpha_0, \alpha_1 \rangle$  is likewise defined syntactically as a pair of length  $\ell$  binary strings. Although simple, that syntax is flexible and possesses significant modeling power by means of tailoring partitioning to application. We concentrate on the abstract level, considering the evolution of a non-overlapping, generational, infinite population model assuming panmixia and no selective pressure. We are not concerned with whether and how partitioning is defined as it is irrelevant to the development.

Following Hardy [Hardy \(1908\)](#), the model  $q^n$  at generation  $n$  is a vector having for component  $q_\alpha^n$  the prevalence of diploid  $\alpha$  (the probability of selecting  $\alpha$  at generation  $n$ , assuming unbiased selection).<sup>\*</sup> Ordered diploid  $\gamma = \langle \gamma_0, \gamma_1 \rangle$  is produced for generation  $n + 1$  according to following procedural description.

Assuming independent selection events:

- From parent  $\alpha$  — selected with probability  $q_\alpha^n$  — obtain gamete  $\gamma_0$
- From parent  $\beta$  — selected with probability  $q_\beta^n$  — obtain gamete  $\gamma_1$

Following Gieringer [Geiringer \(1944\)](#), let the transmission function  $t_\alpha(g)$  be the probability that gamete  $g$  is produced from parental genome  $\alpha$ . It follows from the above that the equation determining the next generation  $q^{n+1}$  is

$$q_\gamma^{n+1} = \sum_{\alpha} q_\alpha^n t_\alpha(\gamma_0) \sum_{\beta} q_\beta^n t_\beta(\gamma_1) \quad (2.1)$$

---

<sup>\*</sup>The representation here is the conceptual equivalent of Hardy's model.

It should be appreciated that the Mendelian [Mendel \(1865\)](#) laws of segregation<sup>†</sup> and independent assortment<sup>‡</sup> need not be respected by the transmission function.

The right hand side of (2.1) is invariant under interchange of the summation variables  $\alpha$  and  $\beta$ , which is equivalent to interchanging  $\gamma_0$  and  $\gamma_1$ . This symmetry reflects the fact that which haploid of  $\gamma$  is designated as  $\gamma_0$  is arbitrary,

$$q_{\langle\gamma_0,\gamma_1\rangle}^{n+1} = q_{\langle\gamma_1,\gamma_0\rangle}^{n+1}$$

The model corresponding to (2.1) is low-level in the sense that it regards  $\langle\gamma_0,\gamma_1\rangle$  and  $\langle\gamma_1,\gamma_0\rangle$  as distinct when  $\gamma_1 \neq \gamma_0$ . A higher-level model based on sets is easily obtained,

$$q_{\{\gamma_0,\gamma_1\}} = \begin{cases} 2q_{\langle\gamma_0,\gamma_1\rangle} & \text{if } \gamma_0 \neq \gamma_1 \\ q_{\langle\gamma_0,\gamma_1\rangle} & \text{otherwise} \end{cases}$$

which is in agreement with Hardy[Hardy \(1908\)](#) (issues he considered and results he obtained relating to invariant distributions for a particular sort of transmission function are not here mentioned because they are irrelevant to the purpose of this section).

## 2.2 Reduction

Evolution equation (2.1) may be reduced to the haploid case. Its right hand side is the product of two summations; denote the first by  $p_{\gamma_0}^{n+1}$  and the second by  $p_{\gamma_1}^{n+1}$  so that

$$q_{\langle\gamma_0,\gamma_1\rangle}^{n+1} = p_{\gamma_0}^{n+1} p_{\gamma_1}^{n+1} \tag{2.2}$$

where for any haploid  $\gamma_0$ ,

$$p_{\gamma_0}^{n+1} = \sum_{\alpha} q_{\alpha}^n t_{\alpha}(\gamma_0) \tag{2.3}$$

---

<sup>†</sup> Alleles of a given locus segregate into separate gametes.

<sup>‡</sup> Alleles of one gene sort into gametes independently of the alleles of another gene.

It suffices to determine the evolution of the distributions  $p^n$ . Uncoupling  $p$  from  $q$  using (2.3), and equation (2.2) with superscript  $n$  — instantiate the  $n$  in (2.2) with  $n - 1$  — yields the evolution equation

$$\begin{aligned} p_{\gamma_0}^{n+1} &= \sum_{\alpha_0, \alpha_1} q_{\langle \alpha_0, \alpha_1 \rangle}^n t_{\langle \alpha_0, \alpha_1 \rangle}(\gamma_0) \\ &= \sum_{\alpha_0, \alpha_1} p_{\alpha_0}^n p_{\alpha_1}^n t_{\langle \alpha_0, \alpha_1 \rangle}(\gamma_0) \end{aligned} \quad (2.4)$$

The  $p^n$  are in fact distributions; summing equation (2.2) with superscript  $n$  yields

$$1 = \sum_{\alpha} q_{\alpha}^n = \sum_{\alpha_0, \alpha_1} p_{\alpha_0}^n p_{\alpha_1}^n = \left( \sum_{\alpha_0} p_{\alpha_0}^n \right)^2$$

Let  $[expression]$  denote 1 if *expression* is true, and 0 otherwise.<sup>§</sup> The weighted count of haploid  $g$  in generation  $n$  is

$$\sum_{\alpha_0, \alpha_1} q_{\langle \alpha_0, \alpha_1 \rangle}^n ([g = \alpha_0] + [g = \alpha_1]) \quad (2.5)$$

$$= \sum_{\alpha_0, \alpha_1} p_{\alpha_0}^n p_{\alpha_1}^n [g = \alpha_0] + \sum_{\alpha_0, \alpha_1} p_{\alpha_0}^n p_{\alpha_1}^n [g = \alpha_1] \quad (2.6)$$

$$= 2p_g^n \quad (2.7)$$

Hence the (normalized) prevalence of haploid  $g$  in generation  $n$  is the  $g$ th component of the distribution  $p^n$ . Moreover, (2.5) and (2.2) show (for  $n > 0$ ) invertibility of the map

$$\pi : \mathbf{q}^n \longmapsto \mathbf{p}^n$$

Evolution equation (2.4) in matrix form is

$$p'_g = p^T M_g p \quad (2.8)$$

---

<sup>§</sup> $[\dots]$  is sometimes referred to as an *Iverson bracket*.



where current state  $p$  (generation  $n$ ) and next state  $p'$  (generation  $n + 1$ ) are column vectors, and the  $g$ th transmission matrix is

$$\left(M_g\right)_{u,v} = t_{\langle u,v \rangle}(g) \quad (2.9)$$

(vectors and matrices are indexed by haploids — length  $\ell$  binary strings).

## 2.3 Specialization

This section summarizes from the development in Vose [Vose \(1999a\)](#). It specializes the haploid evolution equations in the previous section to a context where mask-based crossing over and mutation operators are used, leading to Vose’s infinite population model for Genetic Algorithms. Whereas in previous sections *component* referred to a component of a distribution vector  $q^n$  or  $p^n$ , in this section a component is either a probability (when when speaking of a component of a distribution vector), or a bit (when speaking of a component of a haploid).

The set of haploids (i.e., length  $\ell$  binary strings) is a commutative ring  $\mathcal{R}$  under component-wise addition and multiplication modulo 2. This algebraic structure is crucial to Vose’s specialization and subsequent analysis of [\(2.8\)](#). Denote the additive identity by  $\mathbf{0}$  and the multiplicative identity by  $\mathbf{1}$ , and let  $\bar{g}$  abbreviate  $\mathbf{1} + g$ . Except when explicitly indicated otherwise, operations acting on elements of  $\mathcal{R}$  are as defined in this paragraph.<sup>¶</sup>

## 2.4 Mutation

Mutation simulates effects of error that happen with low probability during duplication of chromosome. Mutation provides mechanism to inject new strings into the

---

<sup>¶</sup>In particular,  $g\bar{g} = \mathbf{0} = g + g$ ,  $g^2 = g$ ,  $g + \bar{g} = \mathbf{1}$  for all  $g \in \mathcal{R}$ .

next generation population which gives *RHS* ability to search beyond the confines of initial population.

Symbol  $\mu$  is used to represent mutation distribution describing the probability  $\mu_i$  with which  $i \in \Omega$  is selected to be a mutation mask.  $\mu : \Omega \rightarrow \Omega$  is nondeterministic mutation function where the result  $\mu(x)$  of applying mutation function on  $x$  is  $x \oplus i$  with probability  $\mu_i$  of distribution  $\mu$  where  $i$  is *mutation mask*. Mutating  $x$  using mutation mask  $i$  alters the bits of  $x$  in those positions the mutation mask  $i$  is 1.  $\mu \in [0, 0.5)$  is regarded as a *mutation rate* which implicitly specifies distribution  $\mu$  according to rule [Vose and Wright \(1998\)](#)

$$\mu_i = (\mu)^{1^T i} (1 - \mu)^{\ell - 1^T i}$$

If  $g$  should mutate to  $g'$  with probability  $\rho$ , let

$$\mu_{g+g'} = \rho$$

Given distribution  $\mu$ , mutation is the stochastic operator sending  $g$  to  $g'$  with probability  $\mu_{g+g'}$ .

Mutation considered is *independent* for all  $j$  and  $k$  which means [Vose and Wright \(1998\)](#)

$$\mu_j = \sum_{k \otimes i = 0} \mu_{i \oplus j} \sum_{k \otimes i = 0} \mu_{i \otimes j}$$

## 2.5 Crossover

Crossover refers to crossing over (also termed recombination) between two chromosomes (strings in our case). Crossover like mutation also provides mechanism for injection of new strings into new generation population. Masked based crossover is used in this document. [Geiringer \(1944\)](#) used crossover mask with probability (distribution) associated with the mask to generate offsprings from parent chromosomes in absence of mutation and selection. Let  $\chi_m$  be probability distribution with which

$m$  is selected to be a crossover mask. Following Geiringer (1944), if crossing over  $u$  and  $v$  should produce  $u'$  and  $v'$  with probability  $\rho$ , let

$$\chi_m = \rho$$

where  $m$  is 1 at components which  $u'$  inherits from  $u$ , and 0 at components inherited from  $v$ . It follows that

$$\begin{aligned} u' &= mu + \overline{m}v \\ v' &= mv + \overline{m}u \end{aligned}$$

Given distribution  $\chi$ , crossover is the stochastic operator which sends  $u$  and  $v$  to  $u'$  and  $v'$  with probability  $\chi_m/2$  for each  $u'$  and  $v'$ .

$\chi$  can be considered as a *crossover rate* that specifies the distribution  $\chi$  given by rule Vose and Wright (1998)

$$\chi_i = \begin{cases} \chi_{c_i} & \text{if } i > 0. \\ 1 - \chi + \chi_{c_0} & \text{if } i = 0. \end{cases}$$

where  $c \in \Lambda$  is referred to as *crossover type*. Classical crossover types include *1-point crossover* and *uniform crossover*. For *1-point crossover*,

$$c_i = \begin{cases} 1/(\ell - 1) & \text{if } \exists k \in (0, \ell). i = 2^k - 1. \\ 0 & \text{otherwise.} \end{cases}$$

and for uniform crossover,  $c_i = 2^{-\ell}$ .

## 2.6 Mixing Matrix

The combined action of mutation and crossover is referred to as *mixing*. The *mixing matrix*  $M$  is the transmission matrix corresponding to the additive identity of  $\mathcal{R}$  is

$$M = M_0$$

Crossover and mutation are defined in a manner respecting arbitrary partitioning and arbitrary linkage to preserve the ability to endow abstract syntax with specialized semantics. Groups of loci can mutate and crossover with arbitrarily specified probabilities as discussed in above sections. For mutation distribution  $\mu$  and crossover distribution  $\chi$ , whether or not  $\mu$  is independent if mutation is performed before crossover, then transmission function can be expressed as [Vose and Wright \(1998\)](#)

$$t_{\langle u, v \rangle}(g) = \sum_{i \in \mathcal{R}} \sum_{j \in \mathcal{R}} \sum_{k \in \mathcal{R}} \mu_i \mu_j \frac{\chi_k + \chi_{\bar{k}}}{2} [k(u + i) + \bar{k}(v + j) = g] \quad (2.10)$$

Here a child gamete  $g$  is produced via mutation and then crossover (which are operators that commute).

The mixing matrix  $M$  is a fundamental object, because (2.10) implies that evolution equation (2.8) can be expressed in the form

$$p'_g = (\sigma_g p)^T M (\sigma_g p) \quad (2.11)$$

where the permutation matrix  $\sigma_g$  is defined by component equations

$$(\sigma_g)_{u, v} = [u + v = g]$$

## 2.7 Walsh Transform

A time series,  $f(t)$ , in terms of a series of Walsh functions  $W(n,t)$  [Beauchamp \(1975\)](#), viz.

$$f(t) = a_0 W_{0,t} + \sum_{n=1}^{N-1} a_n W_{n,t}$$

where  $n$  is an ordering number,  $N$  is number of terms used in Walsh series to express time series and

$$\frac{a_0}{2} = \frac{1}{T} \int_0^T f(t) W_{0,t} dt$$

$$a_n = \frac{1}{T} \int_0^T f(t) W_{n,t} dt$$

Finite discrete Walsh transform pair on  $N$  sampling points,  $x_t$ , can be expressed as [Beauchamp \(1975\)](#)

$$X_n = \frac{1}{N} \sum_{t=0}^{N-1} x_t W_{n,t} \quad (2.12)$$

$$n = 0, 1, 2 \dots N - 1$$

and

$$x_t = \sum_{n=0}^{N-1} X_n W_{n,t}$$

$$t = 0, 1, 2 \dots N - 1$$

The Walsh function series  $W_{n,t}$  can be obtained using Walsh matrix also known as Hadamard matrix of order  $N$ . Walsh matrix or Hadamard matrix is a square matrix of order  $N$  whose coefficients comprise only  $+1$  and  $-1$  and where its rows (and columns) are orthogonal to one another. The Walsh matrix is defined by

$$W_{n,t} = N^{-1/2} (-1)^{n \cdot t}$$

where  $N^{-1/2}$  is normalization factor and  $n \cdot t$  is bitwise dot product of binary representation of number  $n$  and  $t$ .

The matrix is symmetric, i.e.,

$$W_{n,t} = W_{t,n}$$

and it has entries satisfying

$$W_{n,t \oplus k} = N^{1/2} W_{n,t} W_{n,k}$$

The practical importance of this symmetry is that the transform and inverse represent same mathematical operation, hence simplifying the derivation and application of the transform. With the normalized form, *Walsh matrix* is its own inverse, i.e.,

$$W = W^{-1}$$

In the matrix form, given vector  $w$  and matrix  $A$ , let  $\hat{w}$  and  $\hat{A}$  denote the Walsh transform of  $w$  and  $A$  respectively. Then  $\hat{w} = Ww$  and  $\hat{A} = WAW$ . If  $w$  is a row vector, then  $w$  in its Walsh basis  $\hat{w}$  represents  $wW$ .

## 2.8 Walsh Transform Adaptation

The Walsh transform has spectacular ability to unravel the intricacies of mixing. And that is why we adapt Walsh transform methods for computing evolutionary trajectories, which have already been established for Vose's haploid model [Vose and Wright \(1998\)](#). Adaptation of Walsh transformation efficiently models infinite diploid population evolution. This adaptation of Walsh transformation helps in making feasible comparisons between finite and infinite diploid population short-term evolutionary behavior. Recalling evolution equation [\(2.11\)](#), without selection,

specialized to Vose's infinite population model expressed in mixing matrix's term,

$$p'_g = (\sigma_g p)^T M (\sigma_g p)$$

where the permutation matrix  $\sigma_g$  is defined by component equations

$$(\sigma_g)_{u,v} = [u + v = g]$$

In our model, the Walsh matrix  $W$  is defined by component equations

$$W_{u,v} = 2^{-\ell/2} (-1)^{u^T v}$$

where the subscripts  $u, v$  (which belong to  $\mathcal{R}$ ) on the left hand side are interpreted on the right hand side as column vectors in  $\mathbb{R}^\ell$ . Columns of  $W$  form the orthonormal basis — the *Walsh basis* — which simultaneously diagonalizes the  $\sigma_g$ .

A change of basis which simultaneously diagonalizes the  $\sigma_g$  unravels the evolution equation (2.11). Expressed in the Walsh basis (see [Vose and Wright \(1998\)](#)), the mixing matrix takes the form

$$\widehat{M}_{u,v} = 2^{\ell-1} [uv = \mathbf{0}] \widehat{\mu}_u \widehat{\mu}_v \sum_{k \in \overline{u+v} \mathcal{R}} \chi_{k+u} + \chi_{k+v} \quad (2.13)$$

and equation (2.11) takes the form

$$\widehat{p}'_g = 2^{\ell/2} \sum_{i \in g\mathcal{R}} \widehat{p}_i \widehat{p}_{i+g} \widehat{M}_{i,i+g} \quad (2.14)$$

where  $g\mathcal{R} = \{gi \mid i \in \mathcal{R}\}$  (for any  $g \in \mathcal{R}$ ).

The mapping from generation  $n$  to generation  $n + 1$ , determined in natural coordinates by equation (2.8) in terms of the transmission function (2.9), and given in Walsh coordinates by equation (2.14) in terms of the mixing matrix (2.13), is Markovian; the next state  $p'$  depends only upon the current state  $p$ . Let  $\mathcal{M}$  represent

the mixing transformation,

$$p' = \mathcal{M}(p) \quad (2.15)$$

and let  $\mathcal{M}^n(p)$  denote the  $n$ -fold composition of  $\mathcal{M}$  with itself; thus generation  $n + 1$  is described by

$$p^{n+1} = \mathcal{M}^n(p^1)$$

where  $p^1 = \pi(q^1)$ . We have little to say about the matrix of the Markov chain corresponding to the mixing transformation  $\mathcal{M}$ , because it is uncountable; each state is a distribution vector  $p$  describing a population. However, that is not an obstacle to computing evolutionary trajectories; (2.15) can be computed in Walsh coordinates relatively efficiently via (2.13) and (2.14).

## 2.9 Fast Walsh Transform

However, computation of discrete Walsh transform given by equation (2.12) takes  $N^2$  operations (addition or subtraction). An algorithm using matrix factorization techniques is found to perform transformation in  $N \log_2 N$  operations. This algorithm is fast Walsh transform (FWT). Shanks (1969) described FWT algorithm which is analogous to Cooley and Tukey (1965) algorithm for fast Fourier transformation. Shanks assumed walsh function to be periodic with period  $N$ , where  $N$  is an integral power of 2. So a complete orthogonal set will have  $N$  function  $W_{m,n}$  where  $m = 0, 1, 2, \dots, N - 1$  and  $n = 0, 1, 2, \dots, N - 1$ . The first two discrete walsh functions are defined as

$$W_{0,n} = 1 \text{ for } n = 0, 1, 2, \dots, N - 1 \quad (2.16)$$

$$W_{1,n} = \begin{cases} 1 & \text{for } n = 0, 1, 2, \dots, (N/2) - 1. \\ -1 & \text{for } n = N/2, (N/2) + 1, \dots, N - 1. \end{cases} \quad (2.17)$$



Remainder of set can be generated by using multiplicative iterative equation:

$$W_{m,n} = W_{[m/2],2n} \cdot W_{m-2[m/2],n} \quad (2.18)$$

where  $[m/2]$  indicates the integer part of  $m/2$ .

The discrete Walsh functions as defined here are symmetric with respect to the argument  $(m, n)$ . That is,

$$W_{m,n} = W_{n,m}.$$

For real array of length  $N$ , Walsh transform can be defined as

$$F(m) = \sum_{n=0}^{N-1} f(n)W_{m,n}, \text{ where } m = 0, 1, 2, \dots, N-1 \quad (2.19)$$

Similarly, for inverse transform is

$$f(n) = \frac{1}{N} \sum_{m=0}^{N-1} F(m)W_{m,n}, \text{ where } n = 0, 1, 2, \dots, N-1 \quad (2.20)$$

Since walsh functions  $W_{m,n}$  have values either 1 or  $-1$ , computation of (2.19) and (2.20) does not require multiplication. Shanks (1969) derived using (2.18) an algorithm analogous to Cooley-Tukey algorithm that will require  $N \log_2 N$  summations to compute complete Walsh transform. For  $N = 8$  (which can be extended to general case), indices in (2.19) can be replaced with a set which can only have values 0 and 1. That is,

$$m = 4j_2 + 2j_1 + j_0, j_2, j_1, j_0 = 0 \text{ or } 1 \quad (2.21)$$

$$n = 4k_2 + 2k_1 + k_0, k_2, k_1, k_0 = 0 \text{ or } 1 \quad (2.22)$$

Using these new notations,  $W_{m,n}$  becomes  $W(j_2, j_1, j_0; k_2, k_1, k_0)$ . So (2.19) becomes

$$F(j_2, j_1, j_0) = \sum_{k_0=0}^1 \sum_{k_1=0}^1 \sum_{k_2=0}^1 f(k_2, k_1, k_0) \cdot W(j_2, j_1, j_0; k_2, k_1, k_0) \quad (2.23)$$

Here,  $j_2, j_1, j_0$  is binary representation of  $m$ . So, dividing  $m$  by 2 equivalents to shifting binary representation of  $m$  by 1 to the right and dropping fractional bit. That is, if

$$m \leftrightarrow j_2 j_1 j_0$$

then,

$$[m/2] \leftrightarrow 0 j_2 j_1.$$

Similarly, if

$$n \leftrightarrow k_2 k_1 k_0$$

then,

$$2n \leftrightarrow k_2 k_1 k_0 0.$$

An 8-length Walsh function is periodic with period 8. Thus any index (such as  $2n$ ) can be evaluated modulo 8. This is equivalent to deleting any bits above the third bit and we have

$$2n(modulo 8) \leftrightarrow k_1 K_0 0$$

Using these indices, (2.18) becomes

$$W(j_2, j_1, j_0; k_2, k_1, k_0) = W(0, j_2, j_1; k_1, k_0, 0) \cdot W(0, 0, j_0; k_2, k_1, k_0). \quad (2.24)$$

$j_0$  can only be 0 or 1, so  $W(0, 0, j_0; k_2, k_1, k_0)$  represents either  $W_{0,n}$  or  $W_{1,n}$ . The function  $W_{0,n}$  is 1 for all  $n$ . And function  $W_{1,n}$  is 1 if  $0 < n < 4$  and  $W_{1,n}$  is -1.0 if  $4 < n < 7$ . Thus, from (2.22),  $W_{1,n}$  is +1.0 if  $k_2 = 0$  and  $W_{1,n}$  is -1.0 if  $k_2 = 1$ . Therefore,

$$W(0, 0, j_0; k_2, k_1, k_0) = (-1)^{j_0 k_2}. \quad (2.25)$$

(2.24) can be used to factor  $W(0, j_2, j_1; k_1, k_0, 0)$  to get

$$W(0, j_2, j_1; k_1, k_0, 0) = W(0, 0, j_2; k_0, 0, 0) \cdot W(0, 0, j_1; k_1, k_0, 0). \quad (2.26)$$

Using (2.25) and (2.26) in (2.24), we get completely factored expression for the 8-length Walsh function

$$W(j_2, j_1, j_0; k_2, k_1, k_0) = (-1)^{j_2 k_0} (-1)^{j_1 k_1} (-1)^{j_0 k_2}. \quad (2.27)$$

Using (2.27), (2.23) becomes

$$F(j_2, j_1, j_0; k_2, k_1, k_0) = \sum_{k_0=0}^1 (-1)^{j_2 k_0} \sum_{k_1=0}^1 (-1)^{j_1 k_1} \cdot \sum_{k_2=0}^1 (-1)^{j_0 k_2} f(k_2, k_1, k_0). \quad (2.28)$$

We can define

$$A_1(j_0, k_1, k_0) = \sum_{k_2=0}^1 (-1)^{j_0 k_2} f(k_2, k_1, k_0) \quad (2.29)$$

Array  $A_1$  is first set of intermediate calculations to compute  $F(m)$ .  $A_2(j_0, j_1, k_0)$  can be computed from  $A_1$  and final result  $A_3(j_0, j_1, j_2)$  from  $A_2$  for 8-length Walsh transform. However, the order of the values will be in the bit reversed form. It can be generalized for the case  $N = 2^p$  by defining intermediate Walsh transform arrays as

$$A_l(j_0, j_1, \dots, j_{l-1}, k_{p-l-1}, \dots, k_0) = \sum_{k_{p-l}=0}^1 A_{l-1}(j_0, j_1, \dots, j_{l-2}, k_{p-l}, k_{p-l-1}, \dots, k_0) \cdot (-1)^{j_{l-1} k_{p-l}} \quad (2.30)$$

where  $l = 1, 2, \dots, p$  and

$$A_0(k_{p-1}, k_{p-2}, \dots, k_0) = f(k_{p-1}, k_{p-2}, \dots, k_0). \quad (2.31)$$

The general equation for the  $M = 2^P$ -length discrete Walsh function is

$$W(j_{p-1}, j_{p-2}, \dots, j_0; k_{p-1}, k_{p-2}, \dots, k_0) = \prod_{i=0}^{p-1} (-1)^{j_{p-1-i} k_i}.$$

## 2.10 Distance

Let vector  $\mathbf{f}$  represent a finite diploid population; component  $\mathbf{f}_\alpha$  is the prevalence of diploid  $\alpha$ . Let the support  $S_{\mathbf{f}}$  of  $\mathbf{f}$  be the set of diploids occurring in the population represented by  $\mathbf{f}$ ,

$$S_{\mathbf{f}} = \{\alpha \mid \mathbf{f}_\alpha > 0\}$$

Let  $\mathbf{q}$  similarly represent an infinite diploid population (see section 2.1). As points in  $\mathbb{R}^{2^\ell \times 2^\ell}$ , the Euclidean distance between  $\mathbf{f}$  and  $\mathbf{q}$  is

$$\|\mathbf{f} - \mathbf{q}\| = \sum_{\alpha}^{\frac{1}{2}} (\mathbf{f}_\alpha - \mathbf{q}_\alpha)^2$$

Whereas a naive computation of this distance involves  $2^\ell \cdot 2^\ell$  terms, leveraging equation (2.2) can significantly reduce the number of terms involved. Note that

$$\|\mathbf{f} - \mathbf{q}\|^2 = \sum_{\alpha \notin S_{\mathbf{f}}} (\mathbf{f}_\alpha - \mathbf{q}_\alpha)^2 + \sum_{\alpha \in S_{\mathbf{f}}} (\mathbf{f}_\alpha - \mathbf{q}_\alpha)^2 \quad (2.32)$$

Using equation (2.2) —  $\mathbf{q}_\alpha = \mathbf{p}_{\alpha_0} \mathbf{p}_{\alpha_1}$  (suppressing superscripts to streamline notation) — together with the fact that  $\mathbf{f}_\alpha = 0$  in every term of the first sum above, the first sum reduces to

$$\begin{aligned} \sum_{\langle \alpha_0, \alpha_1 \rangle \notin S_{\mathbf{f}}} (\mathbf{p}_{\alpha_0} \mathbf{p}_{\alpha_1})^2 &= \sum_{\langle \alpha_0, \alpha_1 \rangle} (\mathbf{p}_{\alpha_0})^2 (\mathbf{p}_{\alpha_1})^2 - \sum_{\langle \alpha_0, \alpha_1 \rangle \in S_{\mathbf{f}}} (\mathbf{p}_{\alpha_0} \mathbf{p}_{\alpha_1})^2 \\ &= \sum_g (\mathbf{p}_g)^2 - \sum_{\alpha \in S_{\mathbf{f}}} (\mathbf{q}_\alpha)^2 \end{aligned} \quad (2.33)$$

It follows from (2.32) and (2.33) that

$$\begin{aligned}
\|\mathbf{f} - \mathbf{q}\|^2 &= \sum_g (\mathbf{p}_g)^2 + \sum_{\alpha \in S_{\mathbf{f}}} (\mathbf{f}_{\alpha} - \mathbf{q}_{\alpha})^2 - \sum_{\alpha \in S_{\mathbf{f}}} (\mathbf{q}_{\alpha})^2 \\
&= \sum_g (\mathbf{p}_g)^2 + \sum_{\alpha \in S_{\mathbf{f}}} \mathbf{f}_{\alpha} (\mathbf{f}_{\alpha} - 2\mathbf{q}_{\alpha})
\end{aligned} \tag{2.34}$$

which involves  $2^{\ell} + |S_{\mathbf{f}}|$  terms, assuming that  $S_{\mathbf{f}}$  is known as a byproduct of computing  $\mathbf{f}$ .

(2.34) computes distance between finite and infinite population efficiently.

## 2.11 Simplification

The haploid case simplified by equations (2.13) and (2.14) are the consequence of specializing to Vose's infinite population model and computing in the Walsh basis. Time switching between the standard basis and the Walsh basis is negligible; the fast Walsh transform (in dimension  $n$ ) has complexity  $n \log n$  [Shanks \(1969\)](#).

Only one mixing matrix as opposed to  $2^{\ell}$  matrices is needed to compute the next generation; evolution equation (2.14) references the same matrix for every  $g$ , whereas evolution equation (2.8) depends upon a different matrix  $M_g$  for each choice of  $g$ . The matrix is computed by a single sum as opposed to a triple sum; compare equation (2.13) with equation (2.10). Also, the relevant quadratic form is computed with a single sum as opposed to a double sum; computing via (2.14) is linear time in the size of  $g\mathcal{R}$  (for each  $g$ ) as opposed to the quadratic time computation (for each  $g$ ) represented by equation (2.8).

From a computational standpoint, the best-case scenario is where recomputation of the matrices mentioned in the previous paragraph is obviated by sufficient memory. The reduction from  $2^{\ell}$  matrices to one matrix helps significantly in that regard. To demonstrate this advantage in concrete terms, consider genomes of length  $\ell = 14$ . Using  $2^{14}$  matrices each of which contains  $2^{14} \times 2^{14}$  entries of type `double` requires

32 terabytes, whereas the mixing matrix at 2 gigabytes fits easily within the memory of a laptop. Moreover, for a population size of  $N \leq 2^{20}$ , the distance computation described in the previous section reduces the number of terms involved by a factor of  $2^{28}/(2^{14} + 2^N) > 252$ .

## 2.12 Convergence

This section presents a cursory numerical investigation of the convergence of finite diploid population short-term behaviour to that of the infinite diploid population model as described in section 2 (the underlying haploid model for the infinite population case is described in section 2.1).

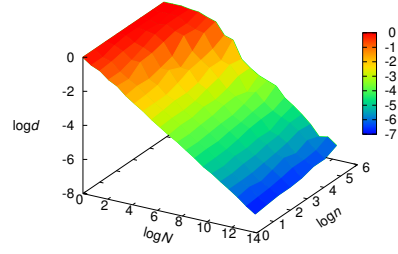
Equations (2.2), (2.13), (2.14), (2.34) were employed to illustrate efficient computation of the distance

$$d = \|\mathbf{f}^n - \mathbf{q}^n\|$$

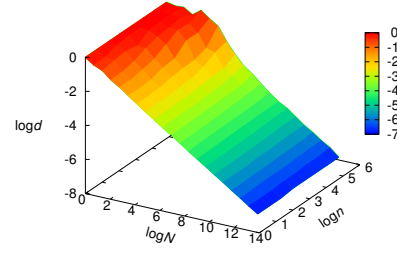
where  $\mathbf{f}^n$  and  $\mathbf{q}^n$  represent finite and infinite diploid populations at generation  $n \in \{1, 2, 4, 8, 16, 32, 64, 128\}$  respectively, beginning from a random initial population ( $\mathbf{f}^0 = \mathbf{q}^0$ ). Genome lengths  $\ell \in \{4, 6, 8, 10, 12, 14\}$  and population sizes  $N = 2^i$  for integer  $0 \leq i \leq 20$  were considered. The crossover distribution  $\boldsymbol{\chi}$  corresponds to independent assortment of bits, and the mutation distribution  $\boldsymbol{\mu}$  corresponds to independent bit mutation probability 0.001,

$$\boldsymbol{\chi}_m = 2^{-\ell}, \quad \boldsymbol{\mu}_g = (0.001)^{\mathbf{1}^T g} (0.999)^{\ell - \mathbf{1}^T g}$$

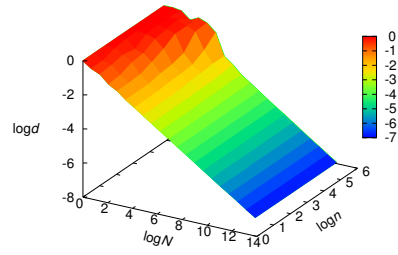
(subscripts above on the left hand side of an equality are interpreted on the right hand side of the equality as column vectors in  $\mathbb{R}^\ell$ ). The finite population case is computed using the itemized procedural definition given in section 2.1; the transmission function (2.10) corresponds to  $\boldsymbol{\mu}$  and  $\boldsymbol{\chi}$  above (bits mutate independently and are freely assorted).



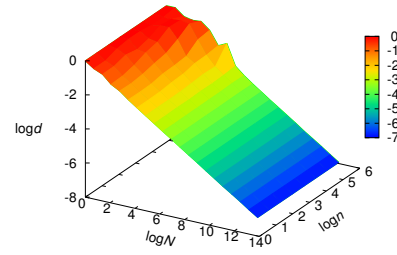
(a)  $\ell = 4$ .



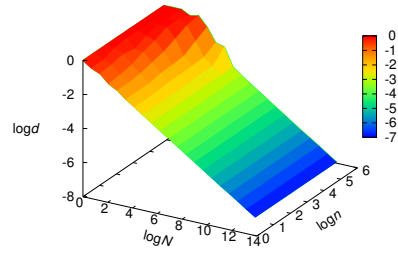
(b)  $\ell = 6$ .



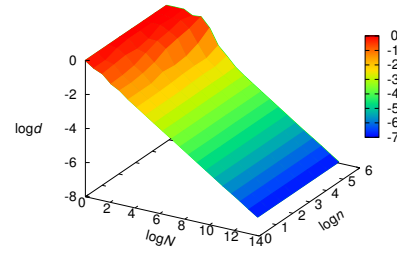
(c)  $\ell = 8$ .



(d)  $\ell = 10$ .



(e)  $\ell = 12$ .



(f)  $\ell = 14$ .

**Figure 2.1: Convergence of finite population behaviour:**  $d$  is distance between finite population  $\mathbf{f}^n$  and infinite population  $\mathbf{q}^n$  at generation  $n$ , population size  $N$ , for genome length  $\ell$  (bits).

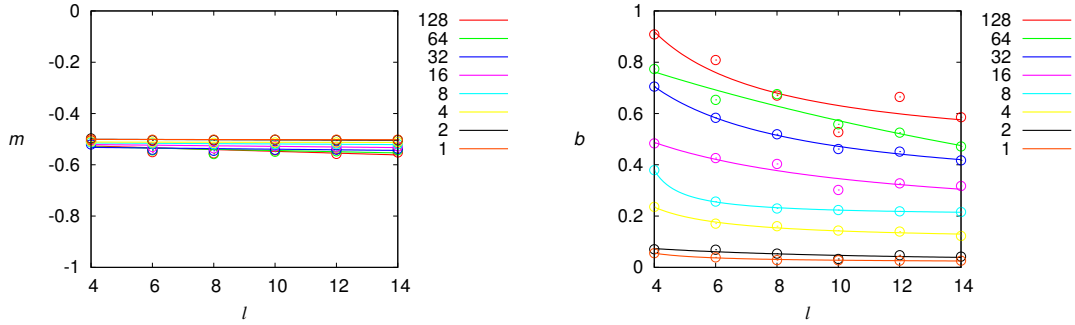
The data, presented in six surface graphs above and organized by genome length, shows a near linear dependence of  $\log d$  on  $\log N$ . As expected, the graphs show

smoothing with increasing genome length (the computation of  $d$  involves averaging over  $\ell$  components), and also with increased population size (as explained in Vose (1999a), the initial transient of a finite haploid population trajectory converges as  $N \rightarrow \infty$  to the corresponding infinite population model).

Of particular interest is the linear trend exhibited above. The slope  $m$  and intercept  $b$  of the regression line

$$\log d = m \log N + b \quad (2.35)$$

was computed using the data above; each was plotted against genome length  $\ell$  and organized by generation  $n$ . The resulting graphs are displayed below.



(a) Slope  $m$ , genome length  $\ell$ .

(b) Intercept  $b$ , genome length  $\ell$ .

**Figure 2.2: Regression parameters:** multi-plot for generation  $n \in \{1, 2, 4, 8, 16, 32, 64, 128\}$ .

Taking the exponential of the regression line (2.35) yields the estimate  $d \approx N^m e^b$ .

Slopes of the regression lines shown in **Figure 2.2** are approximately  $-0.5$ , indicating

$$d \approx k/\sqrt{N}. \quad (2.36)$$



Vose (1999b) calculated variance of next generation population with respect to expected population as

$$\mathcal{E}(\|\mathbf{q} - \mathcal{G}(\mathbf{p})\|^2) = (1 - \|\mathcal{G}(\mathbf{p})\|^2)/N$$

where  $\mathbf{q}$  is actual population and  $\mathcal{G}(\mathbf{p})$  is expected population. Let  $x$  be the random variable  $\|\mathbf{q} - \mathcal{G}(\mathbf{p})\|$ . Let  $\phi$  be the function  $\phi(x) = x^2$  which is convex function. Then  $\mathcal{E}(\|\mathbf{q} - \mathcal{G}(\mathbf{p})\|^2)$  becomes  $\mathcal{E}(\phi(x))$ . From Jensen's Inequality Wikipedia (2016), if  $\phi$  is a convex function, then

$$\begin{aligned}\phi(\mathcal{E}(x)) &\leq \mathcal{E}(\phi(x)) \\ \mathcal{E}(x) &\leq \sqrt{\mathcal{E}(x^2)}\end{aligned}$$

Substituting original variables,

$$\mathcal{E}(\|\mathbf{q} - \mathcal{G}(\mathbf{p})\|) \leq \sqrt{(1 - \|\mathcal{G}(\mathbf{p})\|^2)/N} \quad (2.37)$$

Equation 2.37 shows the expected rate of convergence for the single-step haploid case; the distance is inversely proportional to square root of population size. And equation 2.36 agrees with equation 2.37.

The consistent convergence rate across multiple generations is somewhat surprising, simulation results above indicate it may persist to generation  $n = 128$ .

The intercept graphs above show the constant of proportionality  $k = e^b$  decreases monotonically with genome length  $\ell$ , and increases monotonically with generation  $n$ . The increase in  $k$  for larger  $n$  seems to be a manifestation of the growing nonlinearity uniformly exhibited by the plots in **Figure 2.1** as  $n$  increases. It seems likely that the nonlinearity results from genetic drift experienced by finite populations Crow and Kimura (1970).

# Chapter 3

## Evolutionary Limits

This chapter investigates evolutionary limits predicted by Vose using infinite population model under no selective pressure. It provides computation of predicted limits of infinite population and discusses necessary and sufficient conditions for population to converge in to periodic orbits. Then it studies case of violation in the necessary and sufficient conditions for population to converge periodic orbits.

### 3.1 Limits

Vose states under mild assumptions on mutations (considered later), populations converge under repeated application of  $\mathcal{M}$ . Vose mentions that in general case, periodic orbits are possible but populations converge under repeated application of  $\mathcal{M}^2$  and limits  $\mathbf{p}^* = \lim_{n \rightarrow \infty} \mathcal{M}^{2n}(\mathbf{p})$  and  $\mathbf{q}^* = \lim_{n \rightarrow \infty} \mathcal{M}^{2n+1}(\mathbf{q})$  exist.

Following Vose's theorem, let  $S_g = g\mathcal{R}/\{\mathbf{0}, g\}$ , and let  $|g|$  be the number of non zero bits in  $g$ .

$$\hat{\mathbf{p}}'_g = \begin{cases} 2^{\ell/2} & \text{if } g = 0 \\ x_g \hat{\mathbf{p}}_g + y_g(\hat{\mathbf{p}}_g) & \text{otherwise} \end{cases}$$

where,

$$x_g = 2\widehat{\mathcal{M}}_{g,0}, \quad y_g(z) = 2^{\ell/2} \sum_{i \in S_g} z_i z_{i+g} \widehat{\mathcal{M}}_{i,i+g}.$$

Moreover,

$$\begin{aligned} |g| &= 1 \Rightarrow y_g = 0 \\ |g| &> 0 \Rightarrow |x_g| \leq 1 \\ |x_g| &= 1 \Rightarrow y_g = 0 \end{aligned}$$

With above notations, limits can be expressed in Walsh basis by recursive equations

$$\widehat{\mathbf{p}}^*_g = \begin{cases} (x_g y_g(\widehat{\mathbf{p}}^*) + y_g(\widehat{\mathbf{q}}^*)) / (1 - x_g^2) & \text{if } |x_g| < 0 \\ \widehat{p}_g & \text{otherwise} \end{cases} \quad (3.1)$$

$$\widehat{\mathbf{q}}^*_g = \begin{cases} (x_g y_g(\widehat{\mathbf{q}}^*) + y_g(\widehat{\mathbf{p}}^*)) / (1 - x_g^2) & \text{if } |x_g| < 0 \\ \widehat{\mathcal{M}(\mathbf{p})}_g & \text{otherwise} \end{cases} \quad (3.2)$$

If  $x_g \neq 1$  for all  $g$ , then  $\mathbf{p}^* = \mathbf{q}^* = \lim_{n \rightarrow \infty} \mathcal{M}(\mathbf{p})$  is the limit of mixing. In other cases, mixing converges to a periodic orbit oscillating between  $\mathbf{p}^*$  and  $\mathbf{q}^* = \mathcal{M}(\mathbf{p}^*)$ .

Limits  $\widehat{\mathbf{p}}^*_g$  and  $\widehat{\mathbf{q}}^*_g$  can be computed considering  $g$ th components in order of increasing  $|g|$  and performing complete induction on  $|g|$ . If  $|g| = 0$  then  $g = 0$ . Since  $\widehat{\mathbf{p}}^*_0 = 2^{-\ell/2}$  for all distributions  $\mathbf{p}$ , the 0th components of the sequence  $\mathcal{M}^n(\mathbf{p})$  are identical in the Walsh basis. Since  $|x_0| = 2$  ( $x_g = 2\widehat{\mathcal{M}}_{g,0}$  and  $\widehat{\mathcal{M}}_{0,0} = 1$ ),  $\widehat{\mathbf{p}}^*_g = \widehat{\mathbf{q}}^*_g = 2^{-\ell/2}$ . Next, consider  $|g| = 1$ .  $y_g = 0$  for  $|g| = 0$  (noted from above). These two cases  $|g| < 2$  are base cases for complete induction on  $|g|$ . The inductive hypothesis given by Vose is that for  $|k| < |g|$ , the  $k$ th component of  $\mathcal{M}^n(\mathbf{p})$  in the Walsh basis converges to  $\widehat{\mathbf{p}}^*_k$  or  $\widehat{\mathbf{q}}^*_k$  as  $n \rightarrow \infty$  through even or odd values respectively, and if  $x_k \neq -1$  for all such  $k$ , then  $\widehat{\mathbf{p}}^*_k = \widehat{\mathbf{q}}^*_k$ . And computation of  $y_g(z)$  involves only the  $k$ th components of  $z$  where  $|k| < |g|$ .

Vose gives a necessary and sufficient condition for the sequence

$$p, \mathcal{M}(\mathbf{p}), \mathcal{M}^2(\mathbf{p}), \dots$$

to converge to a periodic orbit as that for some  $g$

$$-1 = \sum_j (-1)^{g^T j} \mu_j = - \sum_{k \in \bar{g}\mathcal{R}} \chi_{k+g} + \chi_k \quad (3.3)$$

## 3.2 Computation of Mutation and Crossover Distribution

Following algorithm installs values of mutation and crossover distributions that satisfies condition described by equation (3.3) for evolutionary sequence to converge in periodic orbits. Let  $\mu_j$  and  $\chi_k$  represent mutation and crossover distributions respectively where  $j, k \in \mathcal{R}$  and  $U01()$  be random number between 0 and 1. For any  $g$  where  $g \in \mathcal{R}$  and  $g \neq 0$ . For all  $j \in \mathcal{R}$ ,

$$\mu_j = \begin{cases} U01() & \text{if } (g^T \cdot j) \text{ is odd.} \\ 0 & \text{otherwise.} \end{cases}$$

This installs some random values in some specific positions in  $\mu$  distribution array according to value of  $g$  and others set to 0. Normalization of  $\mu_j$  gives values for  $\mu$  distribution

$$\mu_j = \mu_j / \sum_{j \in \mathcal{R}} \mu_j$$

such that

$$\sum_{j \in \mathcal{R}} \mu_j = 1.$$

The values  $\mu_j$  satisfy condition (3.3) for  $\mu$  distribution.

Condition  $k \in \bar{g}\mathcal{R}$  in equation (3.3) can be simplified for computation as

$$k = \bar{g}i \text{ where } i \in \mathcal{R}$$

Logical bitwise ANDing both sides by  $\bar{g}$ ,

$$\bar{g}k = \bar{g}\bar{g}i$$

$$\bar{g}k = \bar{g}i$$

$$\bar{g}k = k$$

For all  $k \in \mathcal{R}$ ,

$$\chi_k = U01()$$

$$\chi_{k+g} = U01()$$

where  $k \in \bar{g}\mathcal{R}$ , and

$$\chi_k = 0$$

for other values of  $k$ .

This installs some random values in some specific positions in array of  $\chi$  according to value of  $g$  and others set to 0. Normalization of  $\chi_k$  gives values for *chi* distribution

$$\chi_k = \chi_k / \sum_{k \in \mathcal{R}} \chi_k$$

such that

$$\sum_{k \in \mathcal{R}} \chi_k = 1.$$

The values  $\chi_k$  satisfy condition (3.3) for  $\chi$  distribution.

### 3.3 Initial Population

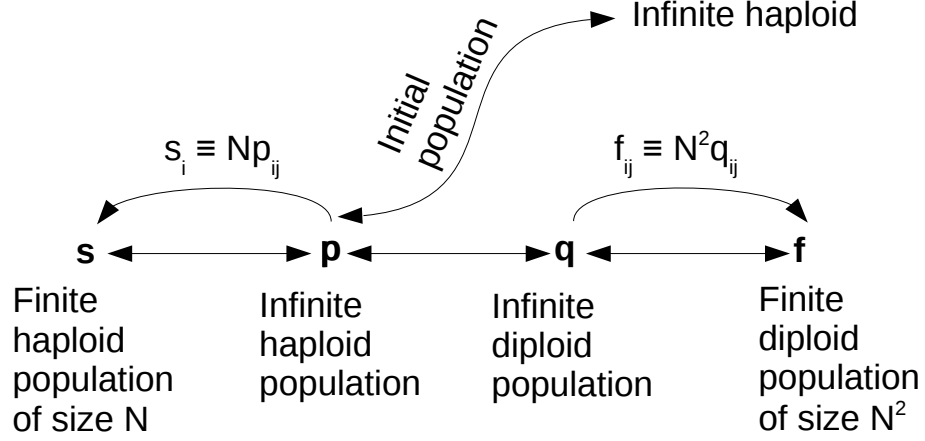


Figure 3.1: Initial population computation

Let finite haploid population  $\mathbf{s}^n$ , finite diploid population  $\mathbf{f}^n$ , infinite haploid population  $\mathbf{p}^n$  and infinite haploid population  $\mathbf{q}^n$  be considered with initial population  $\mathbf{s}^0$ ,  $\mathbf{f}^0$ ,  $\mathbf{p}^0$ ,  $\mathbf{q}^0$  respectively. To investigate oscillating behavior of infinite population evolutionary limits and finite population, same initial population is desired.

For a genome length  $\ell$ , let  $x = 2^\ell$  be number of possible strings in finite haploid population array  $\mathbf{t}$  of population size  $N$ . Possible strings  $\mathbf{t}_i$  are  $0, 1, \dots, x - 1$  where  $i = 0, 1, \dots, N - 1$ . An arbitrary vector  $\mathbf{f}$  of size  $x$  was considered where

$$\mathbf{r}_i = U01(); \quad i = 0, 1, \dots, x - 1$$

and  $U01()$  is random number between 0 and 1. Let  $\mathbf{t}$  represent finite haploid population strings array.

$$\mathbf{t}_j = randp(\mathbf{r}); \quad j = 0, \dots, N - 1$$

where  $\mathbf{t}_j$  is  $j^{th}$  population member and  $randp(\mathbf{r})$  returns random index  $i$  in array  $\mathbf{r}$  with probability  $\mathbf{r}_i$ .

Let  $\mathbf{c}_i$  represent count of haploid member  $i$  in population  $\mathbf{t}$  given by

$$\mathbf{c}_i = \sum_{j=0}^{N-1} [\mathbf{t}_j = i]; \quad i = 0, \dots, x-1 \text{ and } [\dots] \text{ is Iverson bracket.}$$

Then infinite population vector  $\mathbf{p}$  is calculated as

$$\mathbf{p}_i = \frac{\mathbf{c}_i}{\sum_{k=0}^{x-1} \mathbf{c}_k}$$

where  $i = 0, \dots, x-1$  and  $\sum_{k=0}^{x-1} \mathbf{c}_k = N$ .

This  $\mathbf{p}$  is randomly generated initial infinite haploid population vector ( $\mathbf{p}^0$ ) which corresponds to diploid infinite population vector  $\mathbf{q}$  and finite population vectors  $\mathbf{s}$  and  $\mathbf{f}$ .

Finite haploid population members  $\mathbf{t}_j$ s are generated again to match finite haploid population  $\mathbf{s}^0$  with infinite haploid population  $\mathbf{p}^0$ .

$$\mathbf{c}_i = N \cdot \mathbf{p}_i$$

$$\sum_{j=0}^{N-1} [\mathbf{t}_j = i] = \mathbf{c}_i; \quad i = 0, \dots, x-1$$

Initial infinite diploid population  $\mathbf{q}_0$  is calculated corresponding to initial haploid population  $\mathbf{p}^0$  as

$$\mathbf{q}_{i,j} = \mathbf{p}_i \cdot \mathbf{p}_j; \quad i = 0, \dots, x-1; \quad j = 0, \dots, x-1.$$

Let  $\mathbf{v}$  represent finite diploid population member array of size  $N^2$  and  $\mathbf{d}_{i,j}$  represent count of diploid member  $\langle i, j \rangle$  in  $\mathbf{v}$ . Then  $\mathbf{v}$  can be filled with population member to

match initial population vector  $\mathbf{p}$  generating diploid members such that

$$\begin{aligned} \mathbf{d}_{i,j} &= N \cdot \mathbf{p}_i \cdot N \cdot \mathbf{p}_j \\ \sum_{k=0}^{N^2-1} [\mathbf{v}_k = \langle i, j \rangle] &= \mathbf{d}_{i,j} \end{aligned}$$

Finite diploid population vector  $\mathbf{f}$  can be obtained from finite diploid population member array  $\mathbf{v}$  using

$$f_{i,j} = \frac{\mathbf{d}_{i,j}}{\sum_{k=0}^{x-1} \sum_{h=0}^{x-1} \mathbf{d}_{k,h}}$$

where  $i = 0, \dots, x-1$ ,  $h = 0, \dots, x-1$  and  $\sum_{k=0}^{x-1} \sum_{h=0}^{x-1} \mathbf{d}_{k,h} = N^2$ .

This initial infinite haploid population vector  $\mathbf{p}^0$  corresponds to initial infinite diploid population vector  $\mathbf{q}^0$ , initial finite haploid population vector with population size  $N$  and initial finite diploid population vector  $N^2$  with population size  $N^2$ .

### 3.4 Oscillation

Equations (3.1) and (3.2) were implemented with crossover distribution  $\chi$  and mutation distribution  $\mu$  satisfying condition (3.3) to investigate oscillating behavior of predicted infinite population evolutionary limits  $\mathbf{p}^*$  and  $\mathbf{q}^*$  and finite population under no selective pressure.

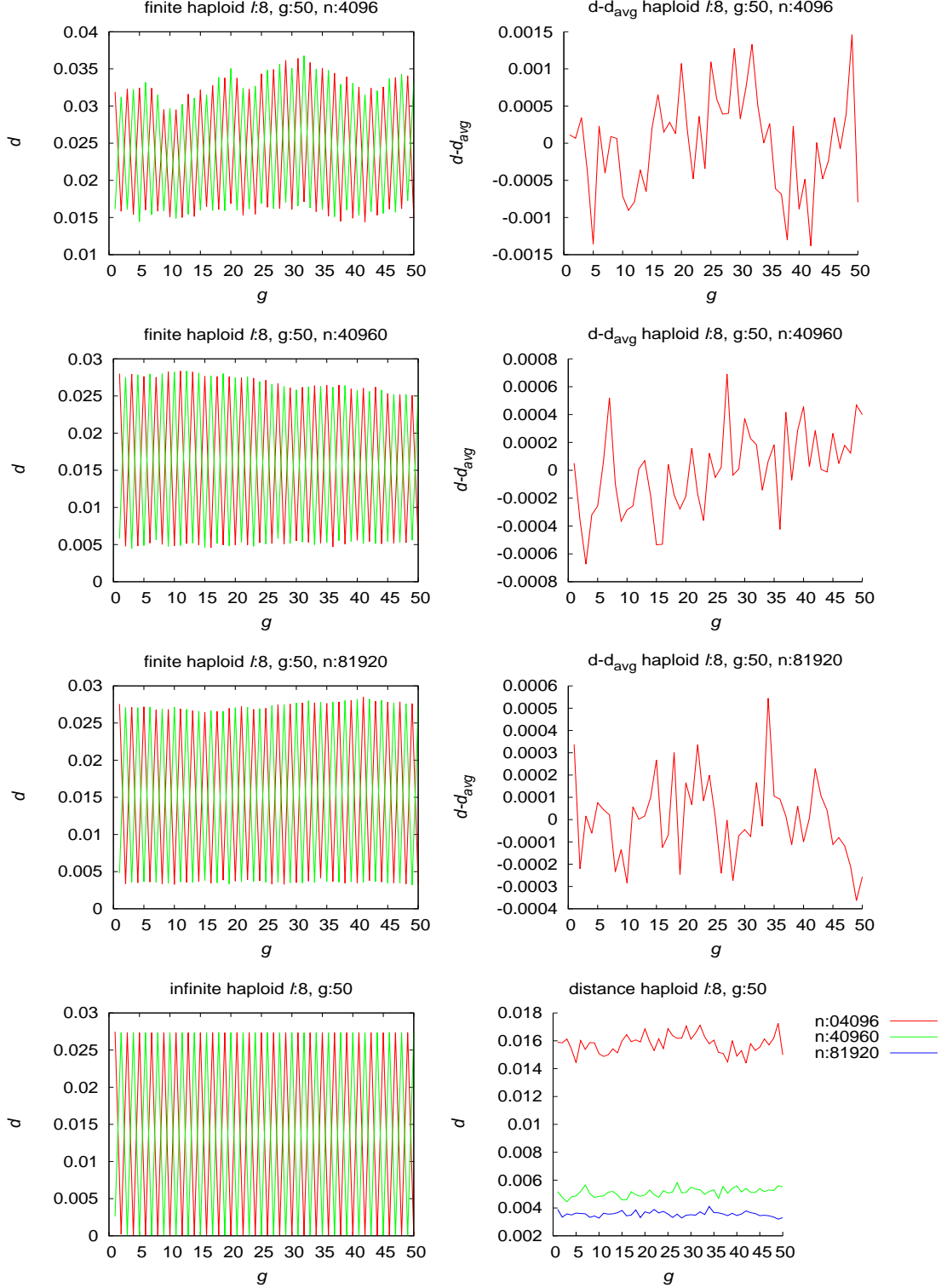
Infinite haploid population evolutionary limits  $\mathbf{p}_h^*$  and  $\mathbf{q}_h^*$  were computed using equations (3.1) and (3.2). Infinite diploid population evolutionary limits  $\mathbf{p}_d^*$  and  $\mathbf{q}_d^*$  as

$$\begin{aligned} \mathbf{p}_{d\langle\gamma_0, \gamma_1\rangle}^* &= \mathbf{p}_{h\gamma_0}^* \mathbf{p}_{h\gamma_1}^* \\ \mathbf{q}_{d\langle\gamma_0, \gamma_1\rangle}^* &= \mathbf{q}_{h\gamma_0}^* \mathbf{q}_{h\gamma_1}^* \end{aligned}$$

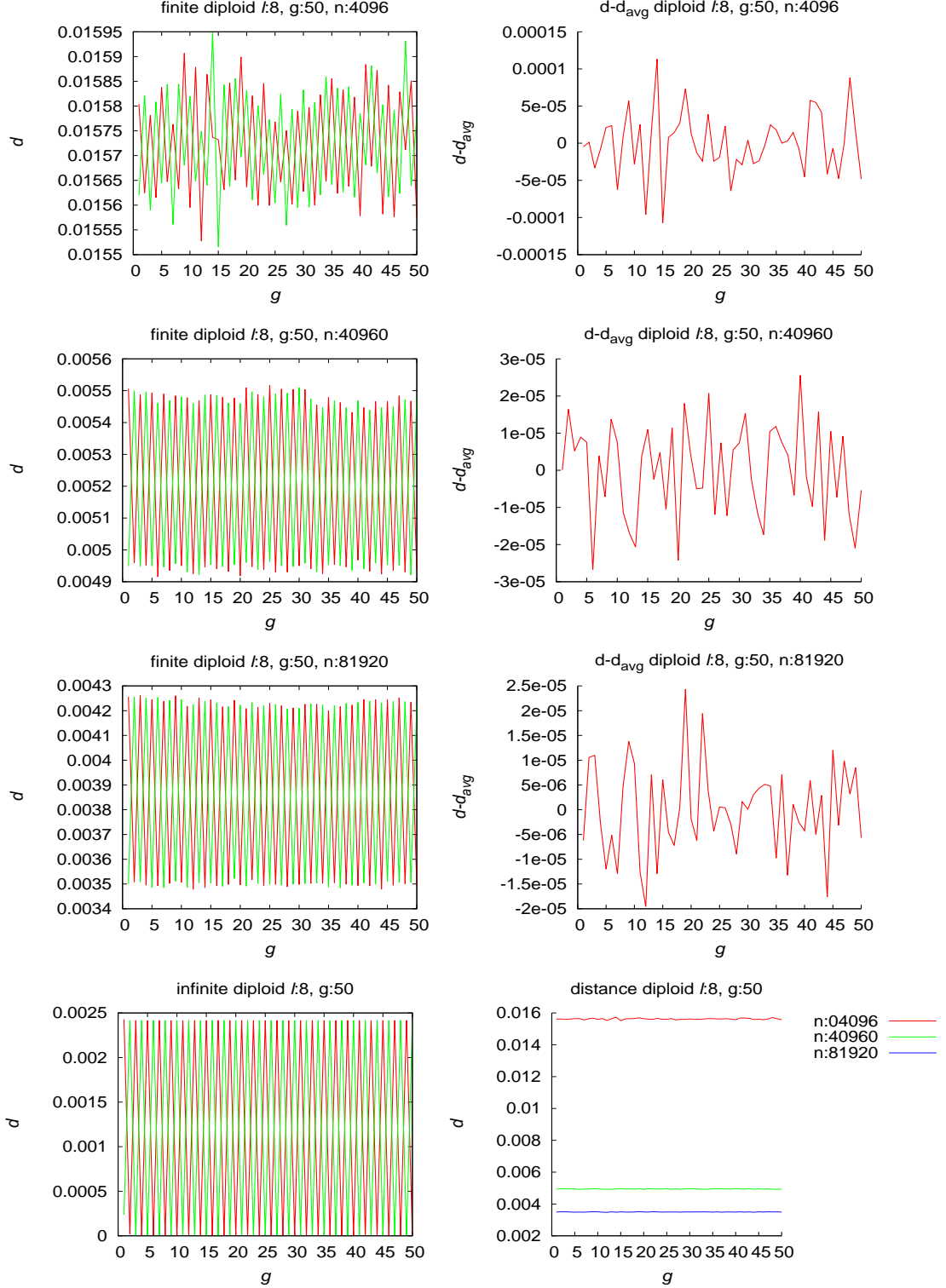
where  $\gamma = \langle \gamma_0, \gamma_1 \rangle$  is diploid genome.



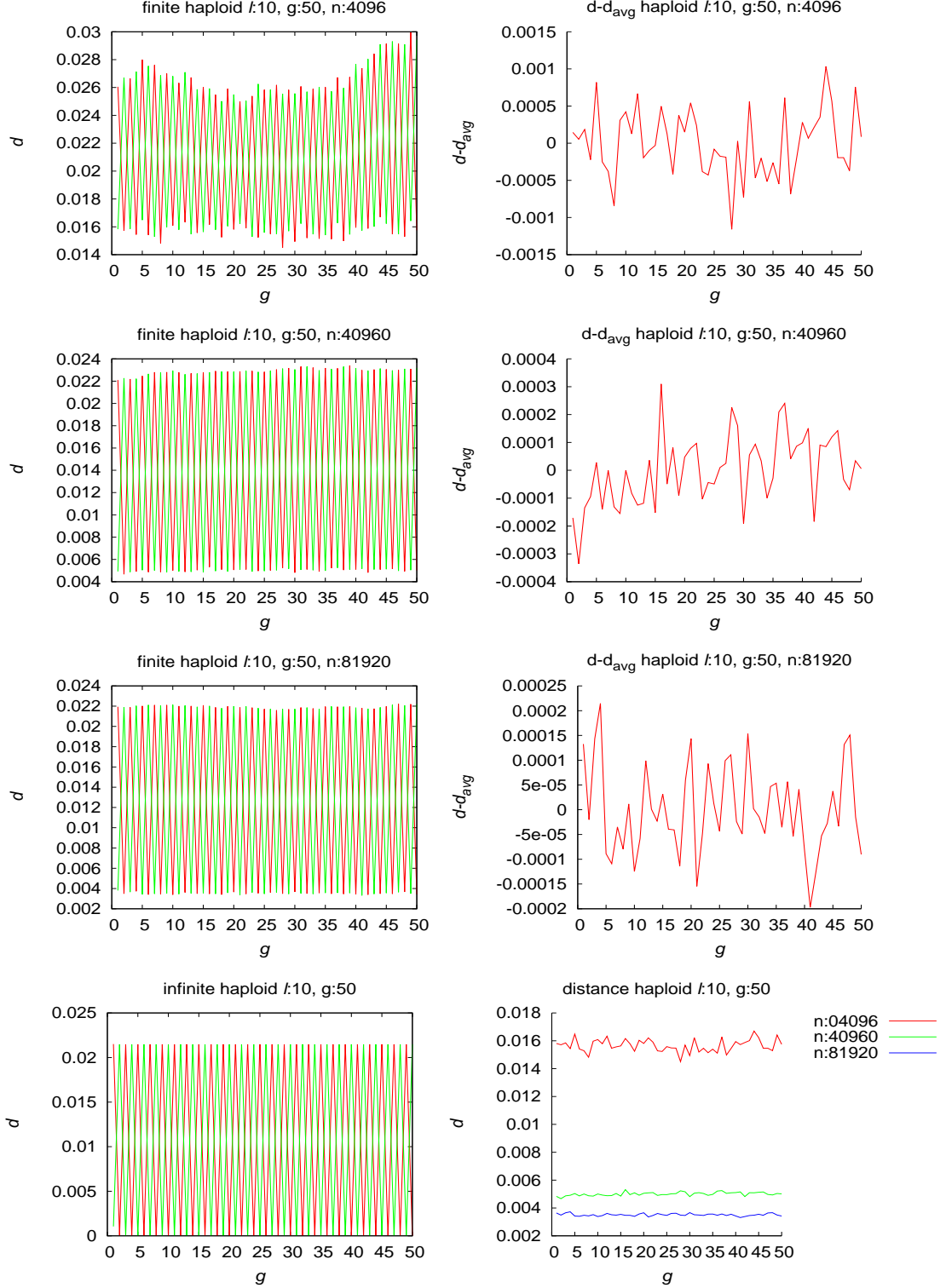
For a genome length  $\ell$ , same initial population (calculated as described in (3.3)) was used for infinite population and all sizes of finite population considered. Genome lengths  $\ell = \{8, 10, 12, 14\}$  were used. Base population size of  $N_0 = 64$  was considered for finite haploid case and different population sizes  $N = \{1N_0^2, 10N_0^2, 20N_0^2\}$  were considered for plotting graphs. The distances of  $\mathbf{p}^n$  and  $\mathbf{s}^n$  to haploid evolutionary limits  $\mathbf{p}_h^*$  and  $\mathbf{q}_h^*$  were plotted and the distances of  $\mathbf{q}^n$  and  $\mathbf{f}^n$  to diploid evolutionary limits  $\mathbf{p}_d^*$  and  $\mathbf{q}_d^*$  were plotted. Distance data of finite population to infinite population were also plotted.



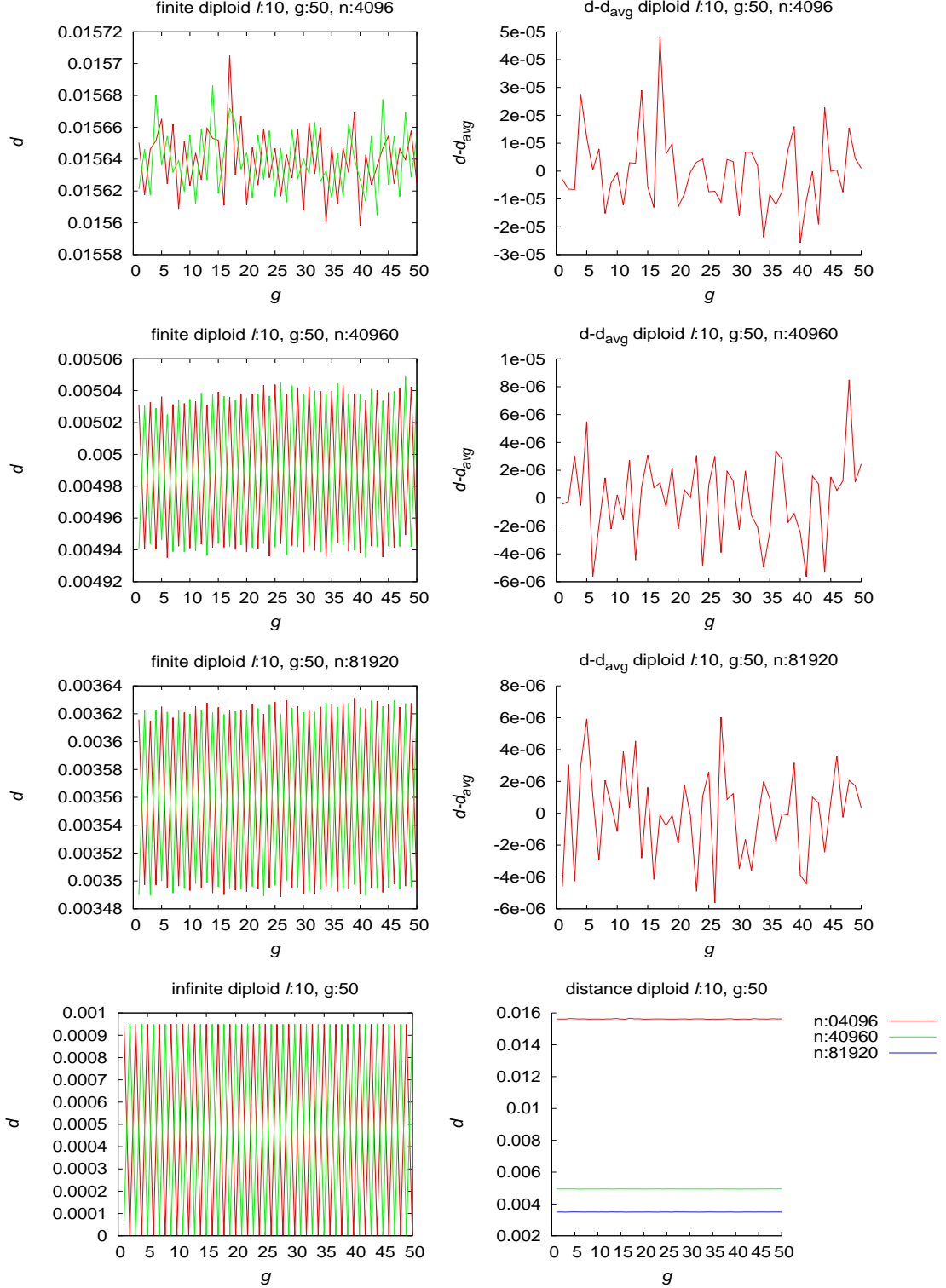
**Figure 3.2: Infinite and finite haploid population oscillation behavior for genome length  $\ell = 8$  (bits):** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limits for  $g$  generations. In right column,  $d$  is distance of finite population to infinite population for  $g$  generations and  $d_{avg}$  is average of distance from 1 to 50 generations.



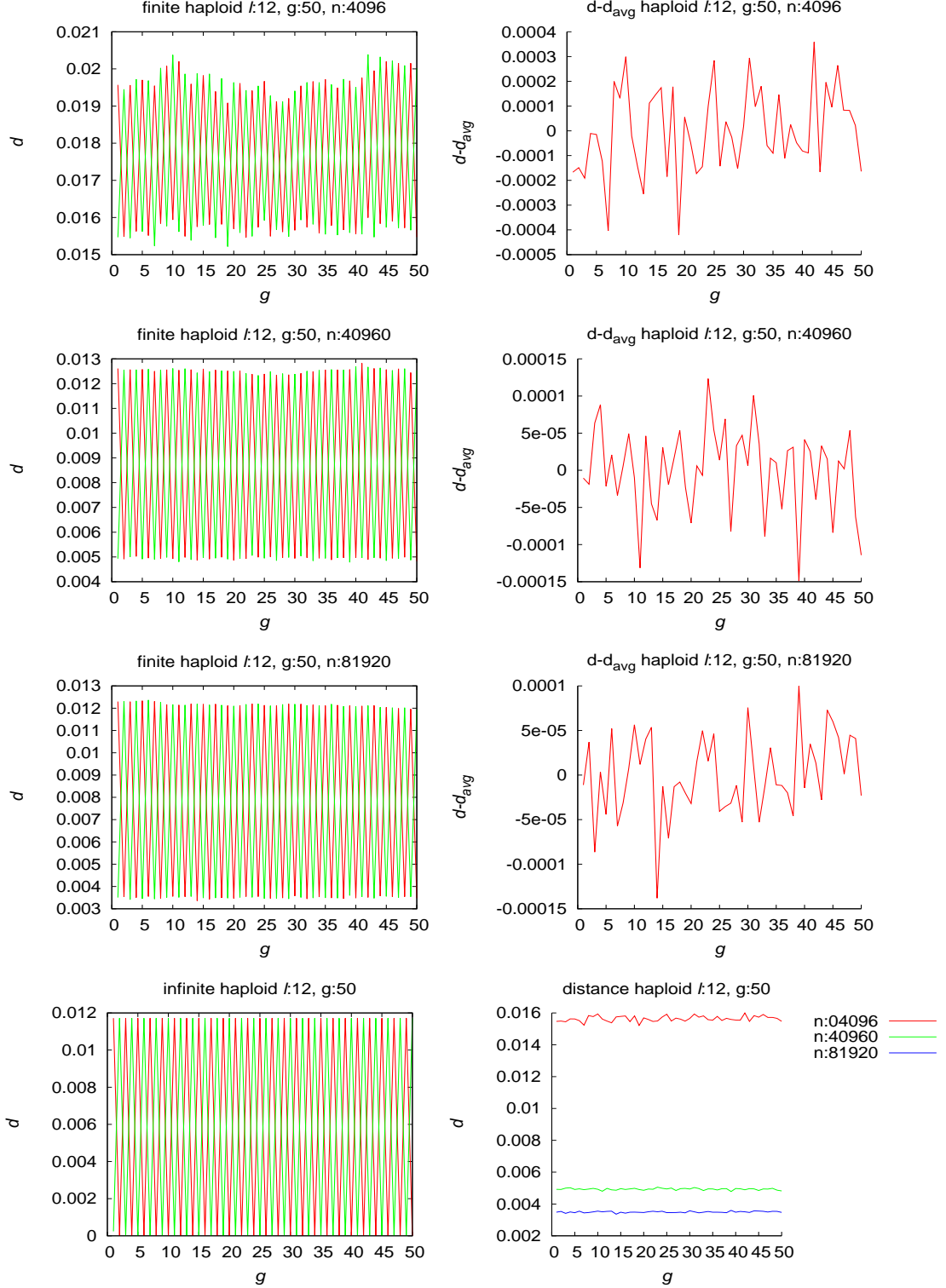
**Figure 3.3: Infinite and finite diploid population oscillation behavior for genome length  $\ell = 8$  (bits):** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limits for  $g$  generations. In right column,  $d$  is distance of finite population to infinite population for  $g$  generations and  $d_{avg}$  is average of distance from 1 to 50 generations..



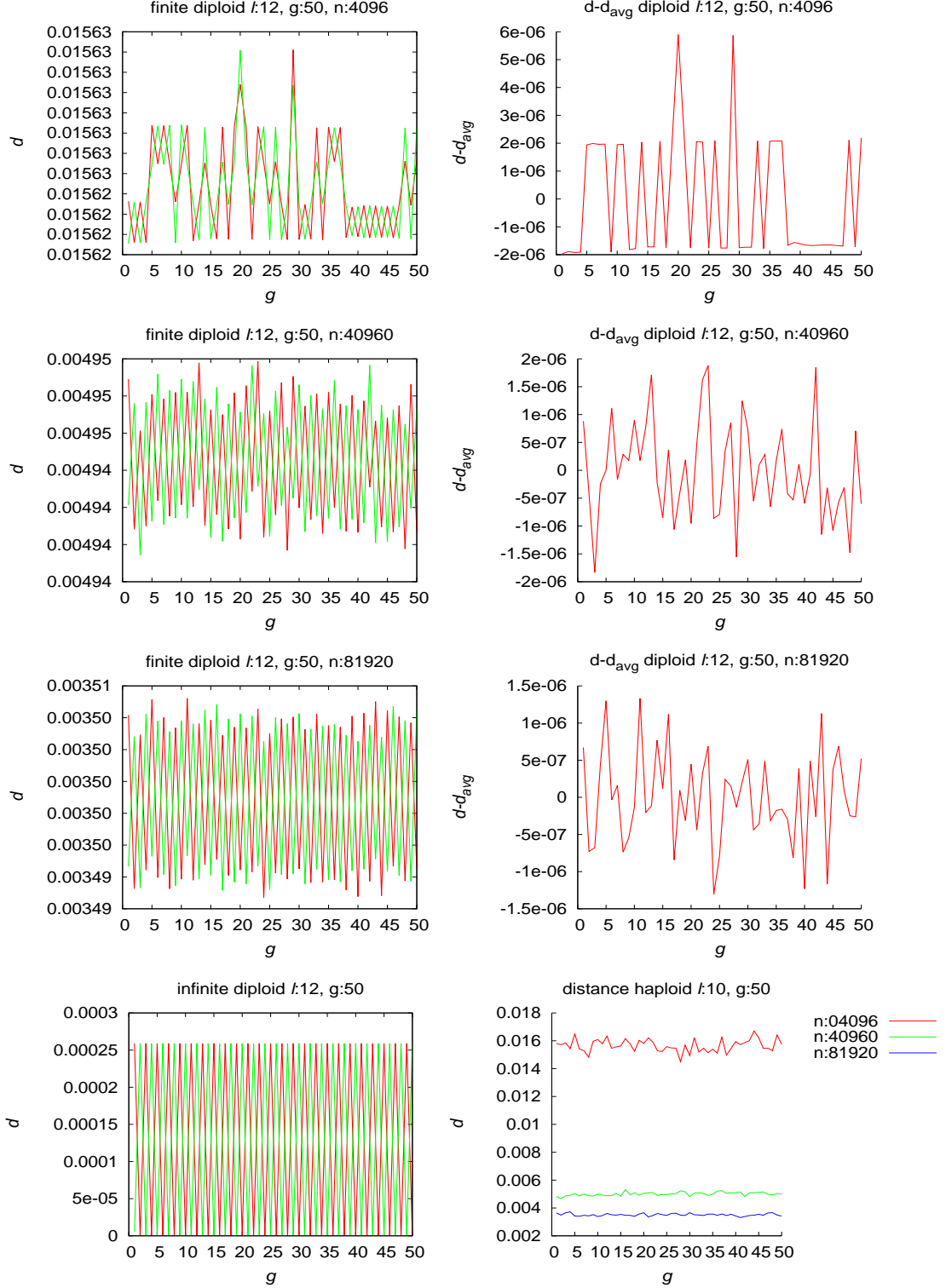
**Figure 3.4: Infinite and finite haploid population oscillation behavior for genome length  $\ell = 10$  (bits):** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limits for  $g$  generations. In right column,  $d$  is distance of finite population to infinite population for  $g$  generations and  $d_{avg}$  is average of distance from 1 to 50 generations..



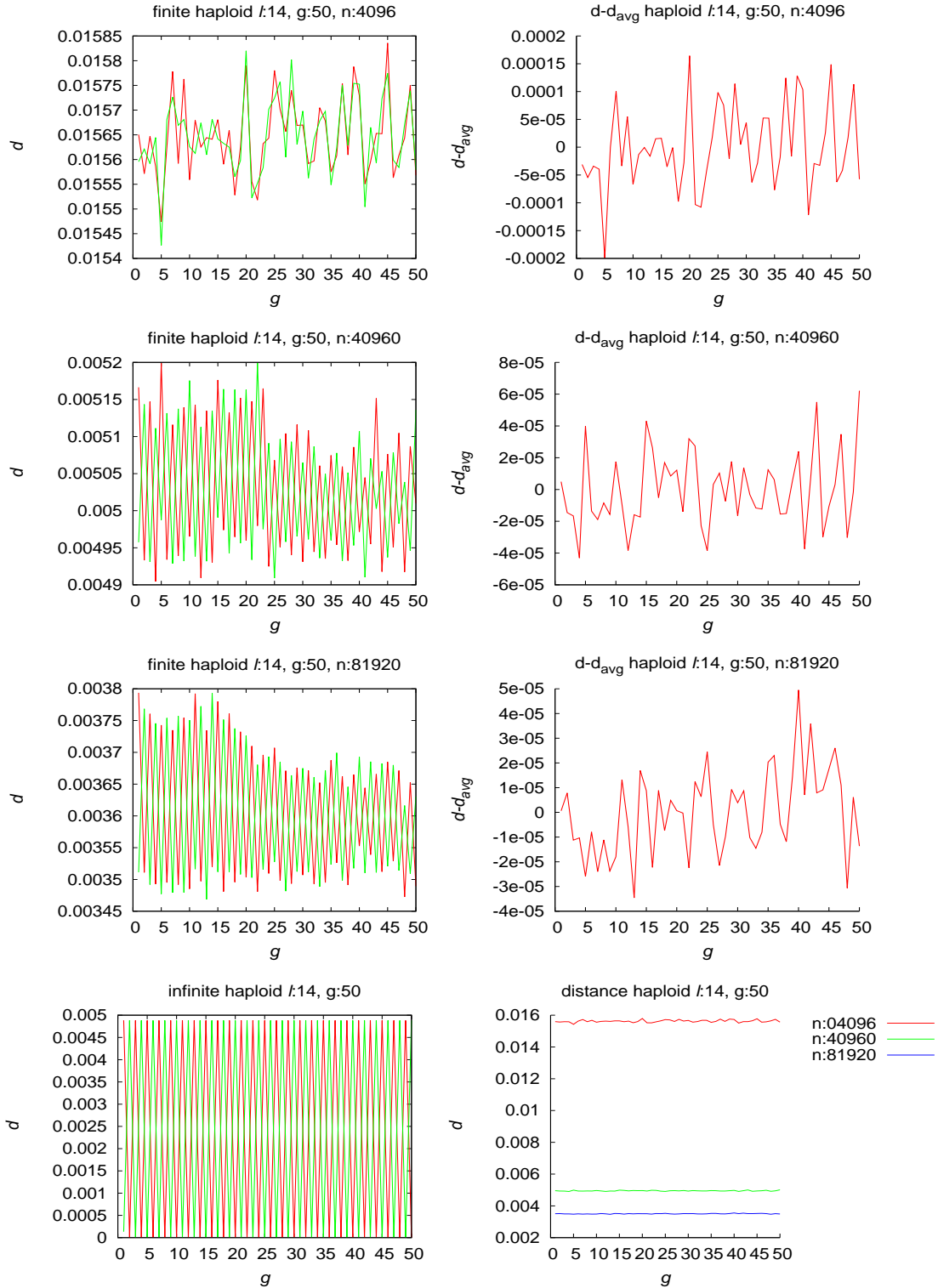
**Figure 3.5: Infinite and finite population oscillation behavior for genome length  $\ell = 10$  (bits):** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limits for  $g$  generations. In right column,  $d$  is distance of finite population to infinite population for  $g$  generations and  $d_{avg}$  is average of distance from 1 to 50 generations..



**Figure 3.6: Infinite and finite haploid population oscillation behavior for genome length  $\ell = 12$  (bits):** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limits for  $g$  generations. In right column,  $d$  is distance of finite population to infinite population for  $g$  generations and  $d_{avg}$  is average of distance from 1 to 50 generations..

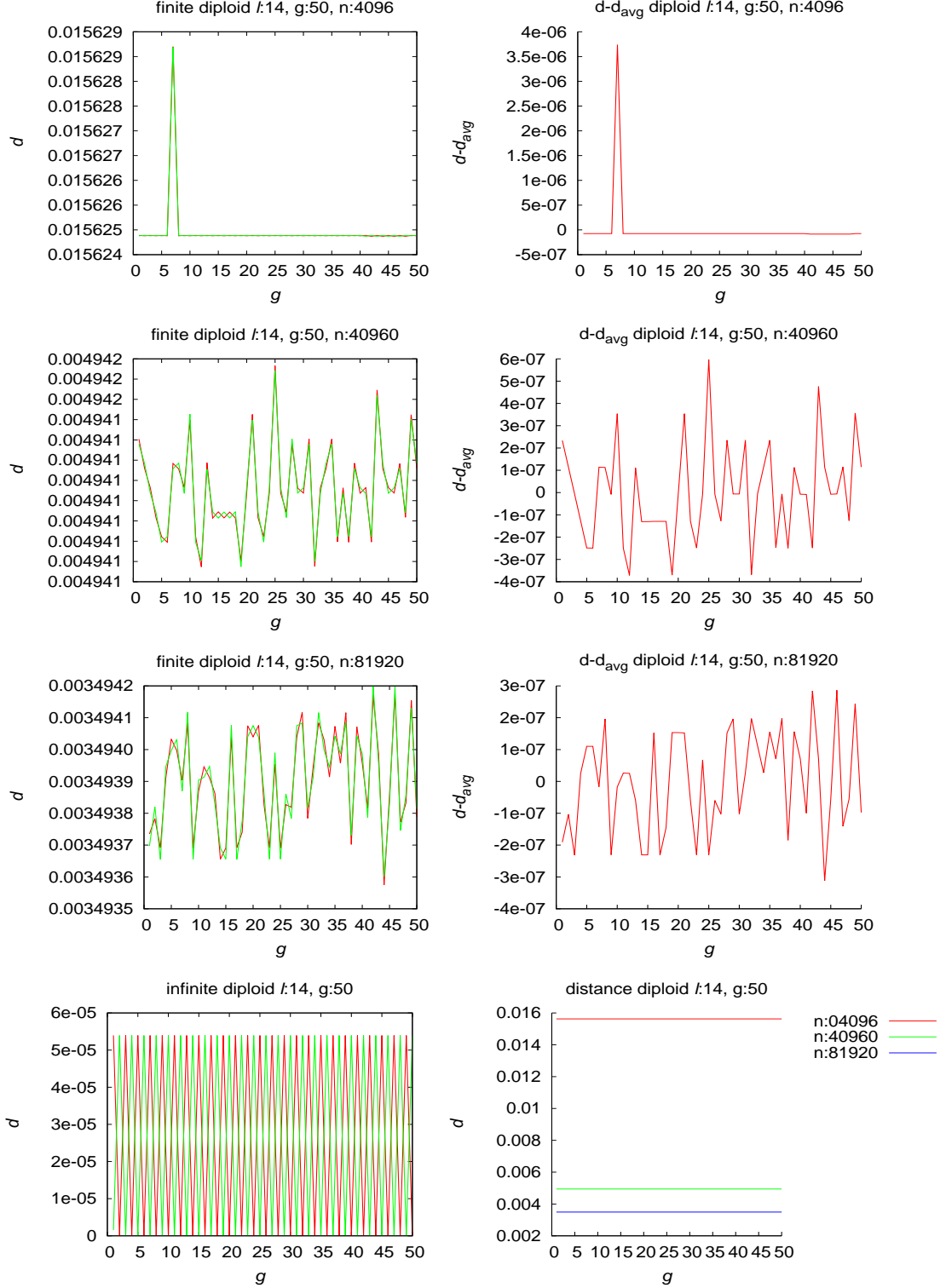


**Figure 3.7: Infinite and finite diploid population oscillation behavior for genome length  $\ell = 12$  (bits):** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limits for  $g$  generations. In right column,  $d$  is distance of finite population to infinite population for  $g$  generations and  $d_{avg}$  is average of distance from 1 to 50 generations..



**Figure 3.8: Infinite and finite haploid population oscillation behavior for genome length  $\ell = 14$  (bits):** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limits for  $g$  generations. In right column,  $d$  is distance of finite population to infinite population for  $g$  generations and  $d_{avg}$  is average of distance from 1 to 50 generations..





**Figure 3.9: Infinite and finite diploid population oscillation behavior for genome length  $\ell = 14$  (bits):** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limits for  $g$  generations. In right column,  $d$  is distance of finite population to infinite population for  $g$  generations and  $d_{avg}$  is average of distance from 1 to 50 generations..

**Figures 3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8 and 3.9** arranged by genome length  $\ell$  and sub-figures within each figures arranged by population size ( $N$ ) for finite population for haploid and diploid population depicts oscillating behavior of both infinite and finite population when necessary and sufficient condition 3.3 is met. Oscillation in finite population in both haploid and diploid case simulation became sharper with increased population size as expected. As size of finite population increased, oscillation behavior depicted by finite population grew analogous to oscillation behavior depicted by infinite population.

Graphs of difference in distance ( $d$ ) and average distance ( $d_{avg}$ ) were plotted for both haploid and diploid cas on right side of oscillation graphs in above figures where  $d$  is distance of finite population to infinite population and  $d_{avg}$  is average of distance from 1<sup>st</sup> to 50<sup>th</sup> generation. For a given genome length  $\ell$  and haploid or diploid case, single graph for distances of different finite population sizes ( $N = 1N_0^2, 10N_0^2, 20N_0^2$ ) were plotted. The resulting graphs showed distance decreased as population size increased which is expected and in congruence with results from section 2.1. Graphs show curve of distance of finite population to infinite population smoothens as population size increased. The graphs of  $d - d_{avg}$  shows decrease in amplitude of ripples as population size increases.

Numerator  $\sqrt{(1 - \|\mathcal{G}(\mathbf{p})\|^2)}$  in equation 2.37 is calculated using initial population and is  $\approx 1$ . So from 2.37, the expected single step distance between finite and infinite population,  $d$ , can be approximated as

$$d \approx 1/\sqrt{N}$$

where  $N$  is size of finite population. Then mathematical expection of single step distance for finite population size  $N = \{4096, 40960, 81920\}$  considered for plotting is shown in following table.

**Table 3.1: Expected single step distance  $d$  for population size  $N$** 

$N$	4096	40960	81920
$d$	0.015625	0.004941	0.003494

Data obtained from distances of finite population of size  $N = \{4096, 40960, 81920\}$  to infinite population obtained from simulation for oscillation for both haploid and dioploid case with genome length  $\ell = \{8, 10, 12, 14\}$  are tabulated below.

**Table 3.2: Experimental distance measured for oscillation:**  $N$  is finite population size,  $\ell$  is genome length and  $\{d', d'', d'''\}$  are distances to infinite population from finite population of sizes  $\{4096, 40960, 81920\}$ 

case	$\ell$	$d'$	$d''$	$d'''$
haploid	8	0.015785	0.005123	0.003559
	10	0.015663	0.005007	0.003511
	12	0.015638	0.004933	0.003497
	14	0.015626	0.004948	0.003503
diploid	8	0.015623	0.004942	0.003498
	10	0.015624	0.004941	0.003494
	12	0.015625	0.004941	0.003494
	14	0.015625	0.004941	0.003494

From table 3.2, averaged distances obtained for finite population size  $N = \{4096, 40960, 81920\}$  are  $\{0.015651, 0.004972, 0.003506\}$  respectively. The results from table 3.2 shows the distance between finite population and infinite population, although measured over number of generations, follows closely the expected single step distance between finite and infinite population given by table 3.1 and the distance decreased as  $1/\sqrt{N}$ .

### 3.5 Violation

The results showed when  $\chi$  and  $\mu$  distributions satisfies (3.3), oscillation occurs in both infinite and finite population. Error  $\epsilon$  was introduced to  $\mu$  distribution and  $\chi$  distribution such that (3.3) did not satisfy anymore and  $x_g \neq 1$  for all  $g$  ( $x_g$  and  $g$  defined in 3.1) so that  $\mathbf{p}^* = \mathbf{q}^*$ .

$\mu$  distribution was treated with  $\epsilon$  such that

$$\mu_i = (1 - \epsilon)\mu_i; \quad i = \{0, 1, 2, \dots, 2^\ell - 1\}.$$

So that sum of  $\mu$  distribution becomes,

$$1 - \epsilon = \sum_{i=0}^{2^\ell-1} \mu_i$$

Then set

$$\mu_0 = \epsilon$$

$\chi$  distribution was treated with  $\epsilon$  such that

$$\chi_i = (1 - \epsilon)\chi_i; \quad i = \{1, 2, \dots, 2^\ell - 1\}$$

So that

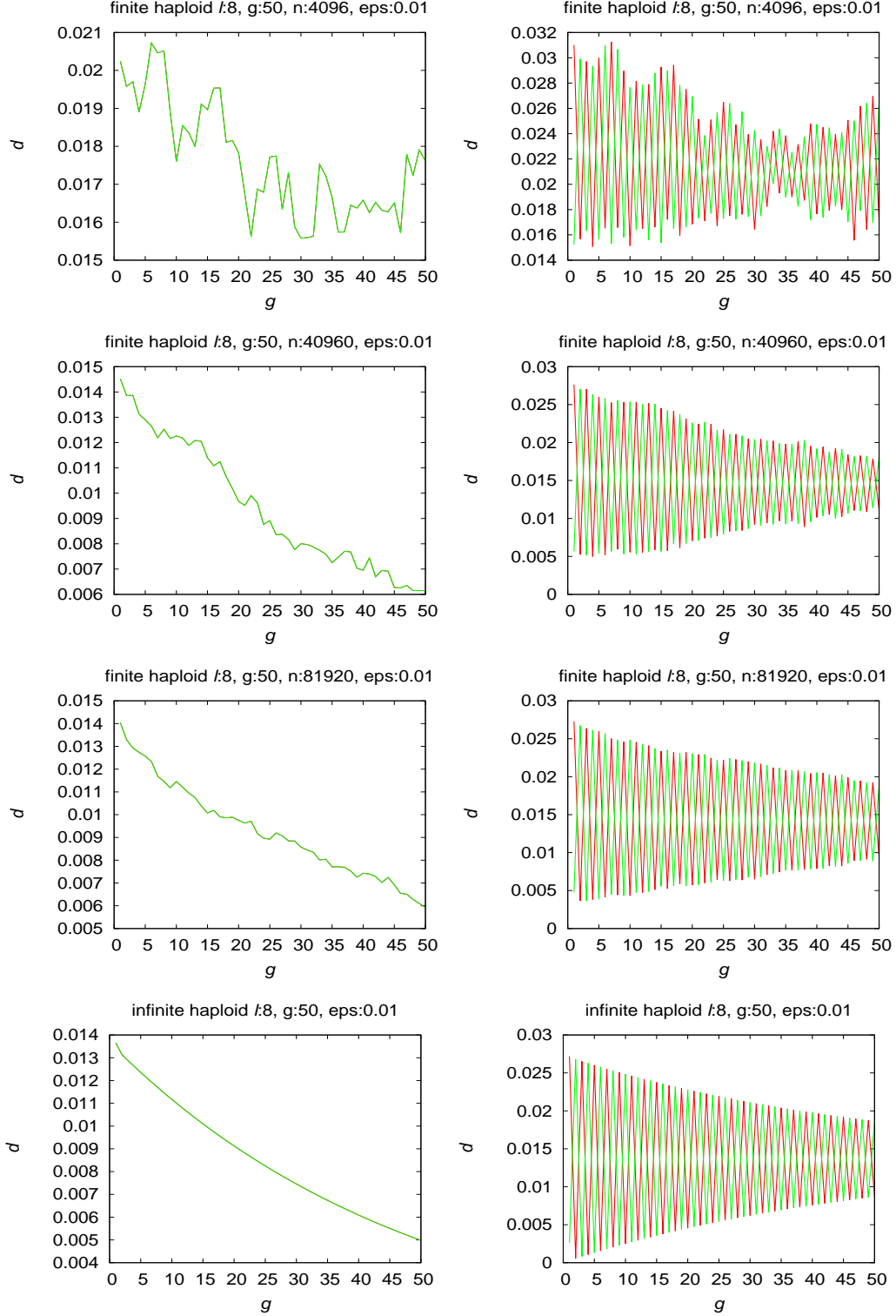
$$\chi_i + \chi_{i+g} = 1 - \epsilon; \quad g \text{ is defined in section 3.1}$$

Then  $j$  is chosen where  $\chi_j = 0$  and set  $\chi_j = \epsilon$ .

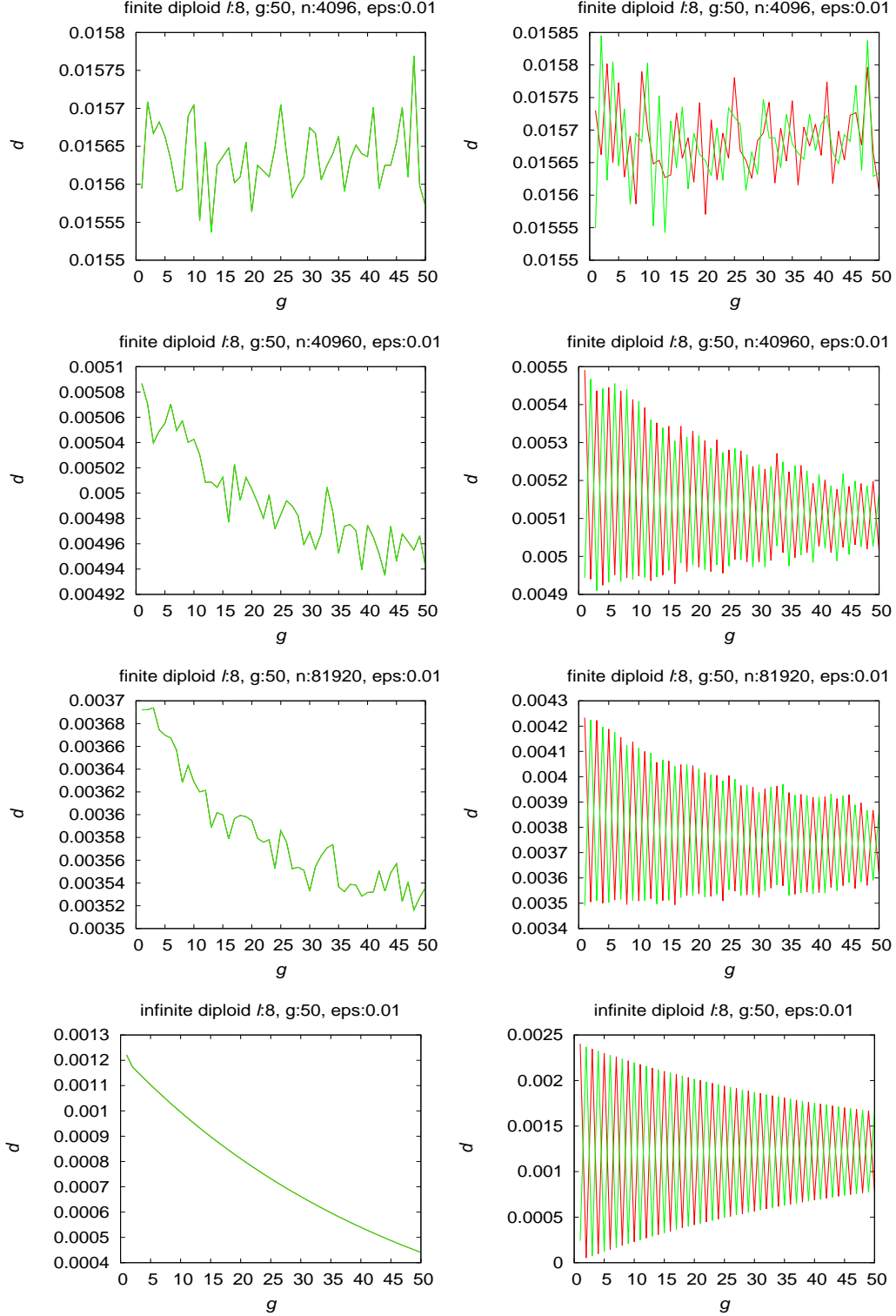
Simulations were run again with violations in (3.3) implemented. Genome lengths  $\ell = \{8, 10, 12, 14\}$  were considered. Different finite haploid population sizes  $N = \{1N_0^2, 10N_0^2, 20N_0^2\}$  were considered.

Let  $\mathbf{p}1^*$  and  $\mathbf{q}1^*$  be evolutionary limits with violation, then  $\mathbf{p}1^* = \mathbf{q}1^* = \mathbf{z}^*$ ;  $\mathbf{z}^*$  is limit when there is violation. The distances of  $\mathbf{p}^n$  and  $\mathbf{s}^n$  to  $\mathbf{z}^*$  were plotted and the

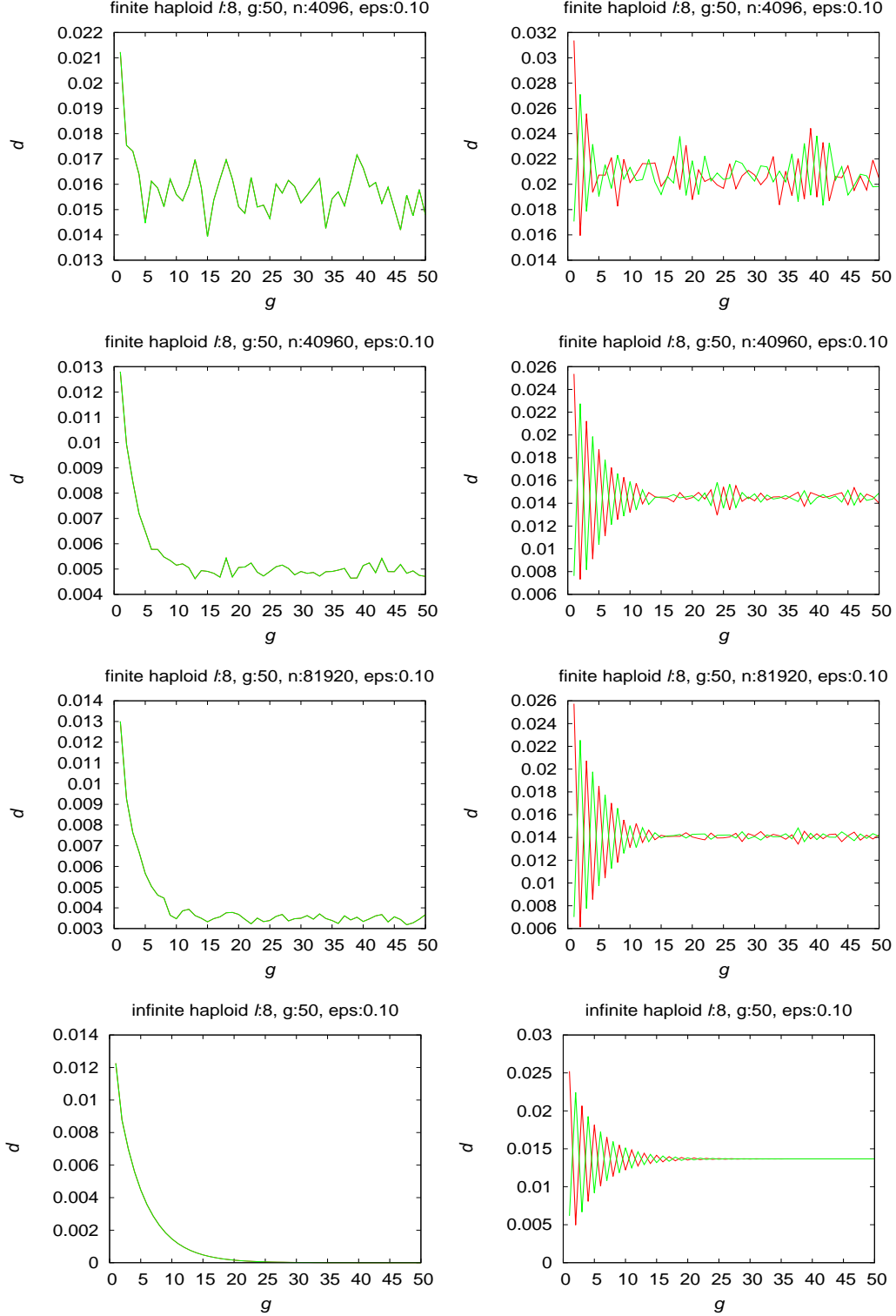
distances of  $\mathbf{q}^n$  and  $\mathbf{f}^n$  to  $\mathbf{z}^*$  were plotted from 1<sup>st</sup> to 50<sup>th</sup> generations. The distances of population to evolutionary limits that would be without violation in  $\boldsymbol{\mu}$  and  $\boldsymbol{\chi}$  were also plotted from 1<sup>st</sup> to 50<sup>th</sup> generations.



**Figure 3.10: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 8$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

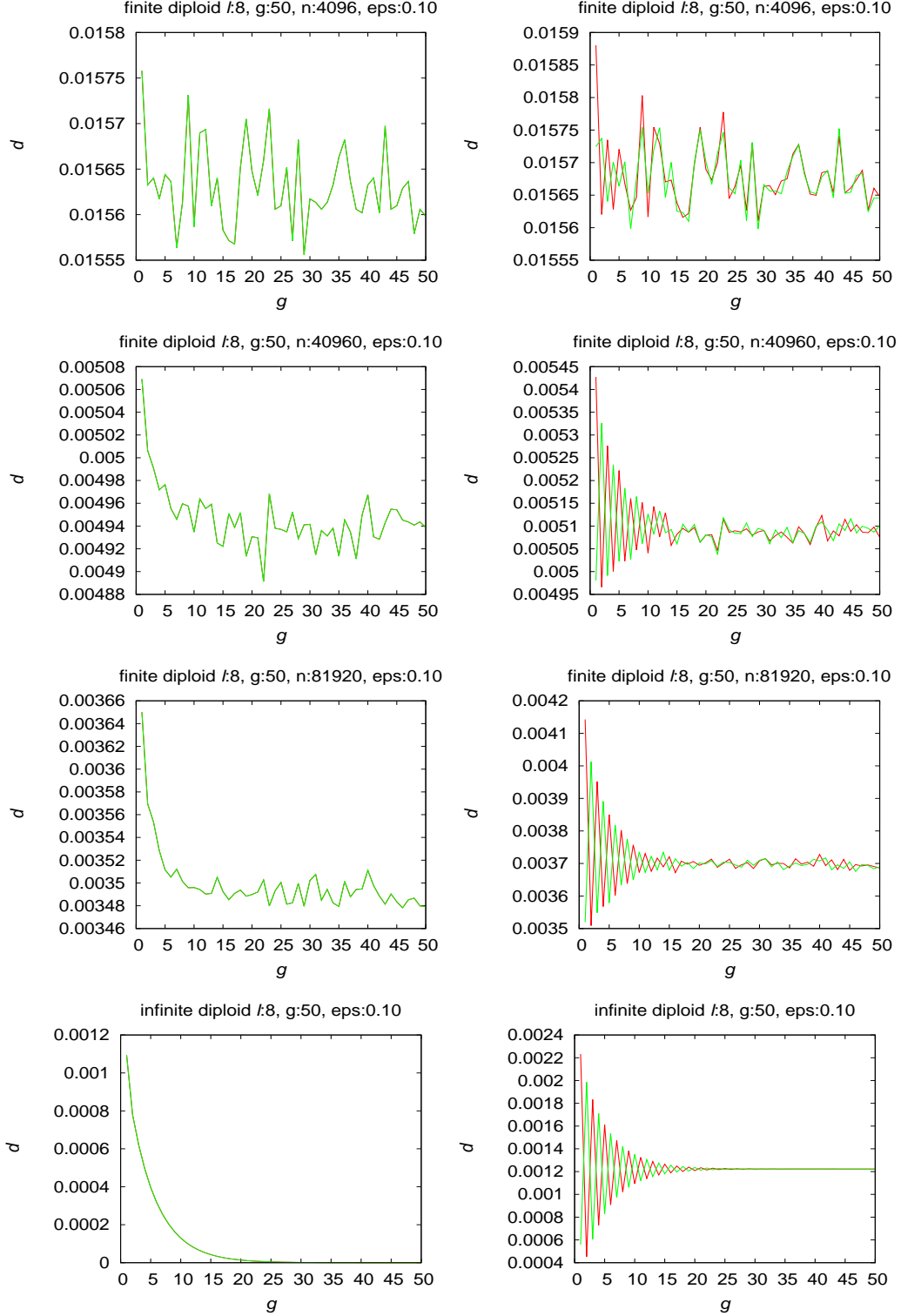


**Figure 3.11: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 8$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

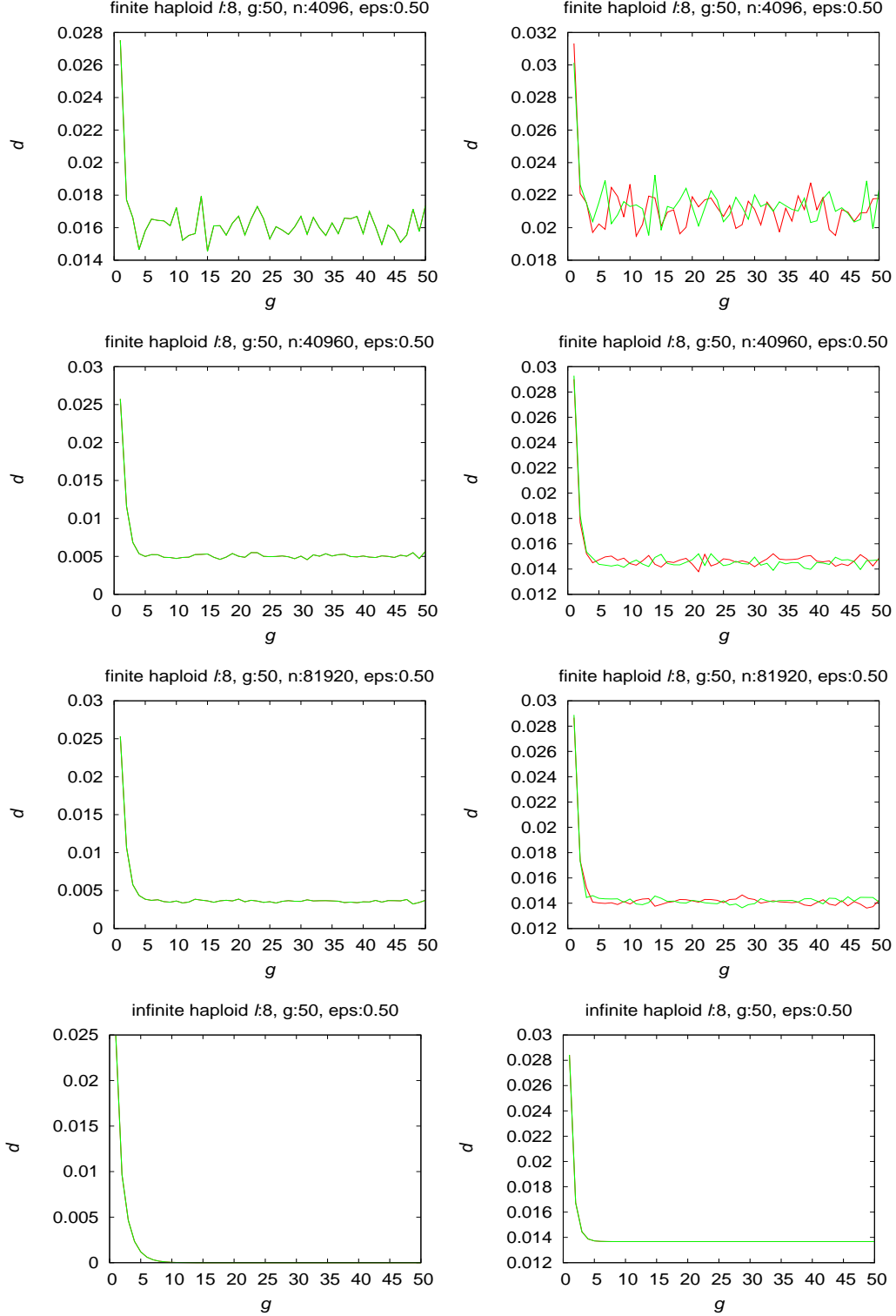


**Figure 3.12: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 8$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

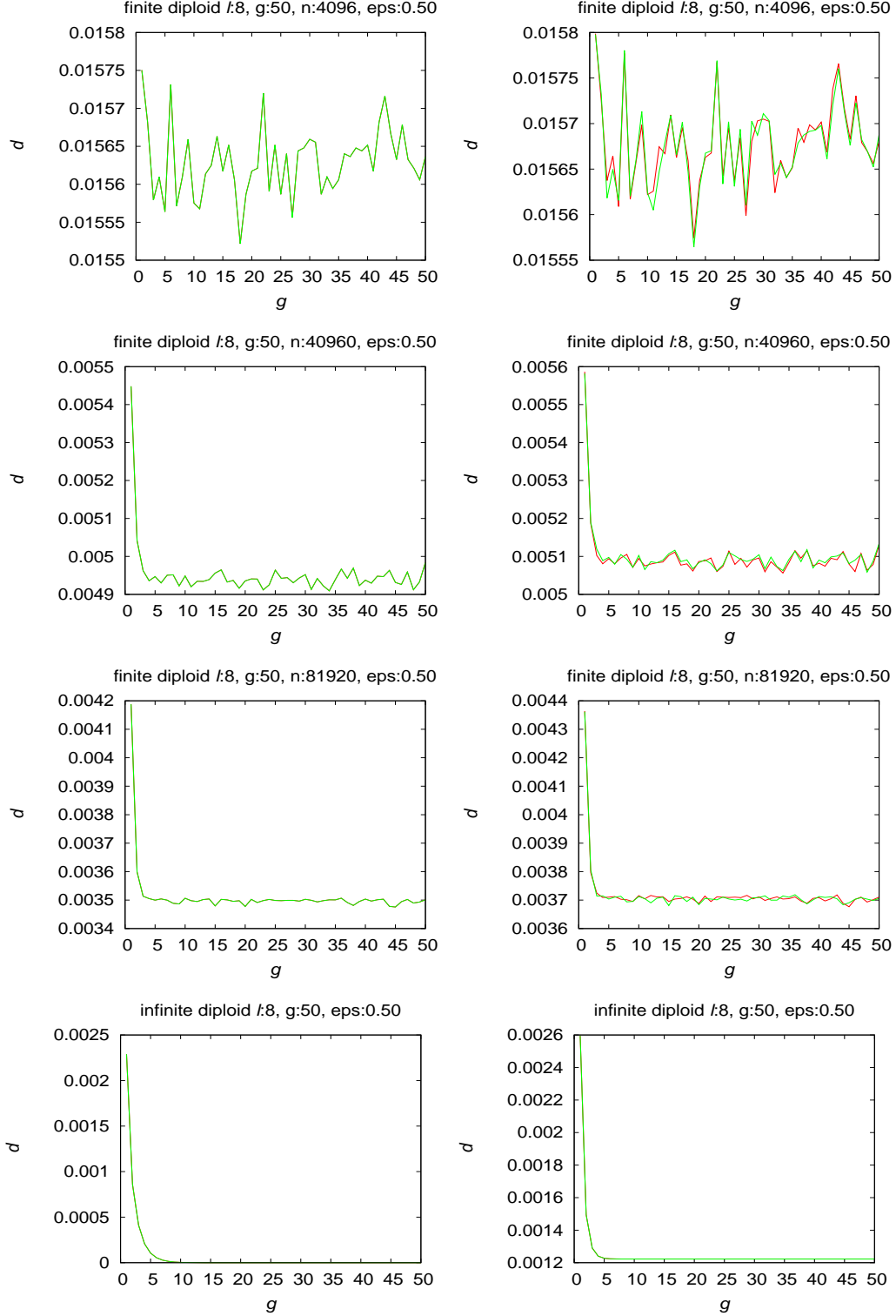




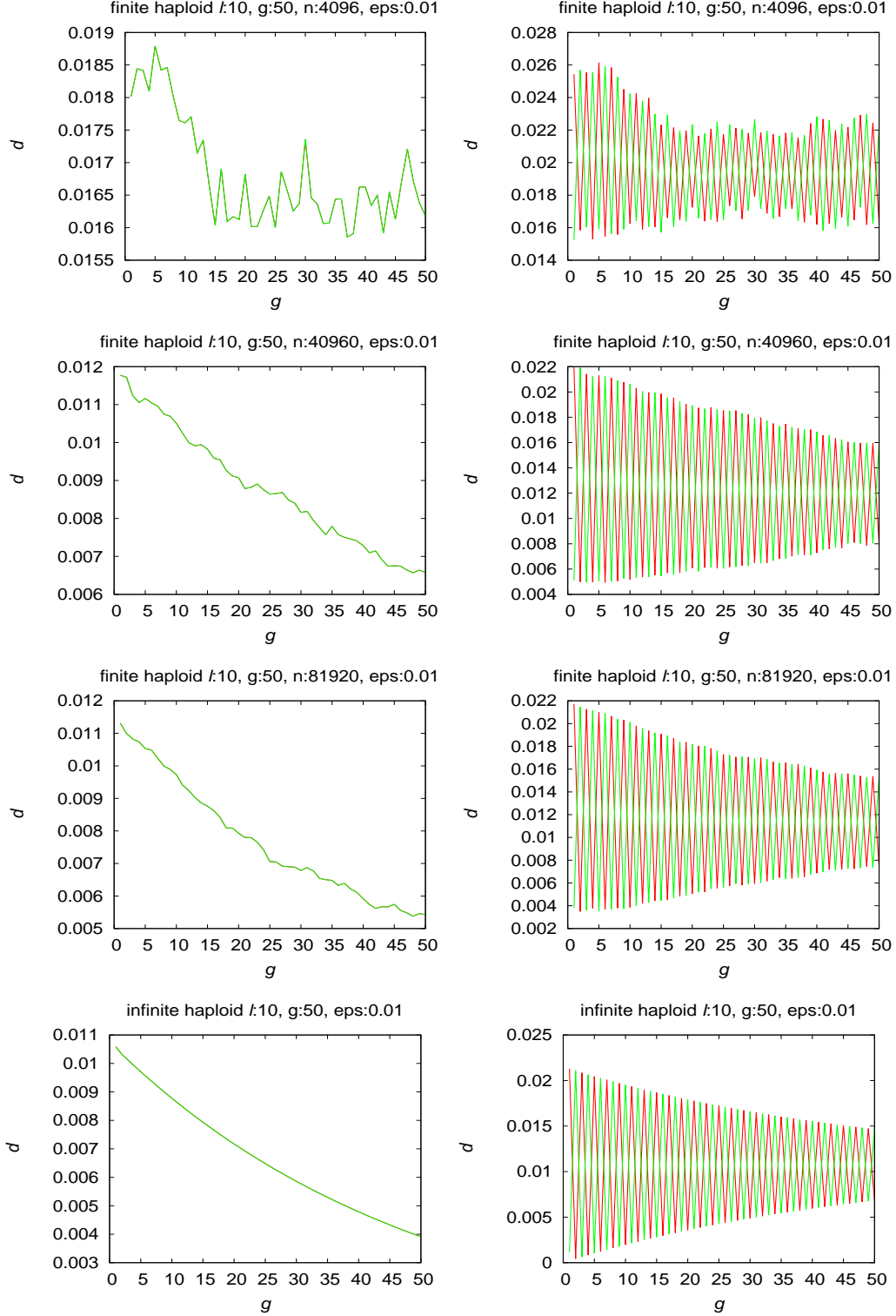
**Figure 3.13: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 8$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



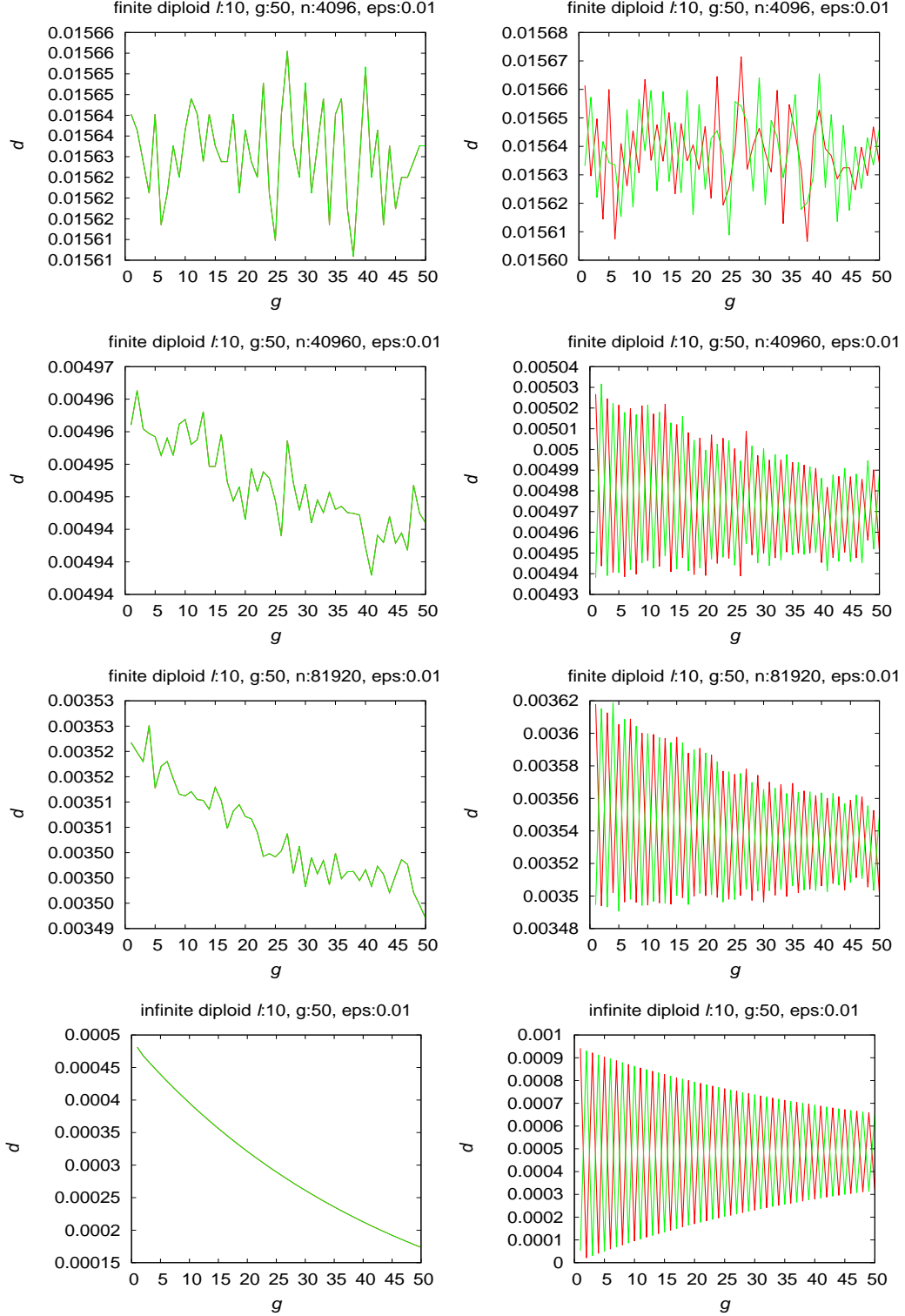
**Figure 3.14: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 8$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



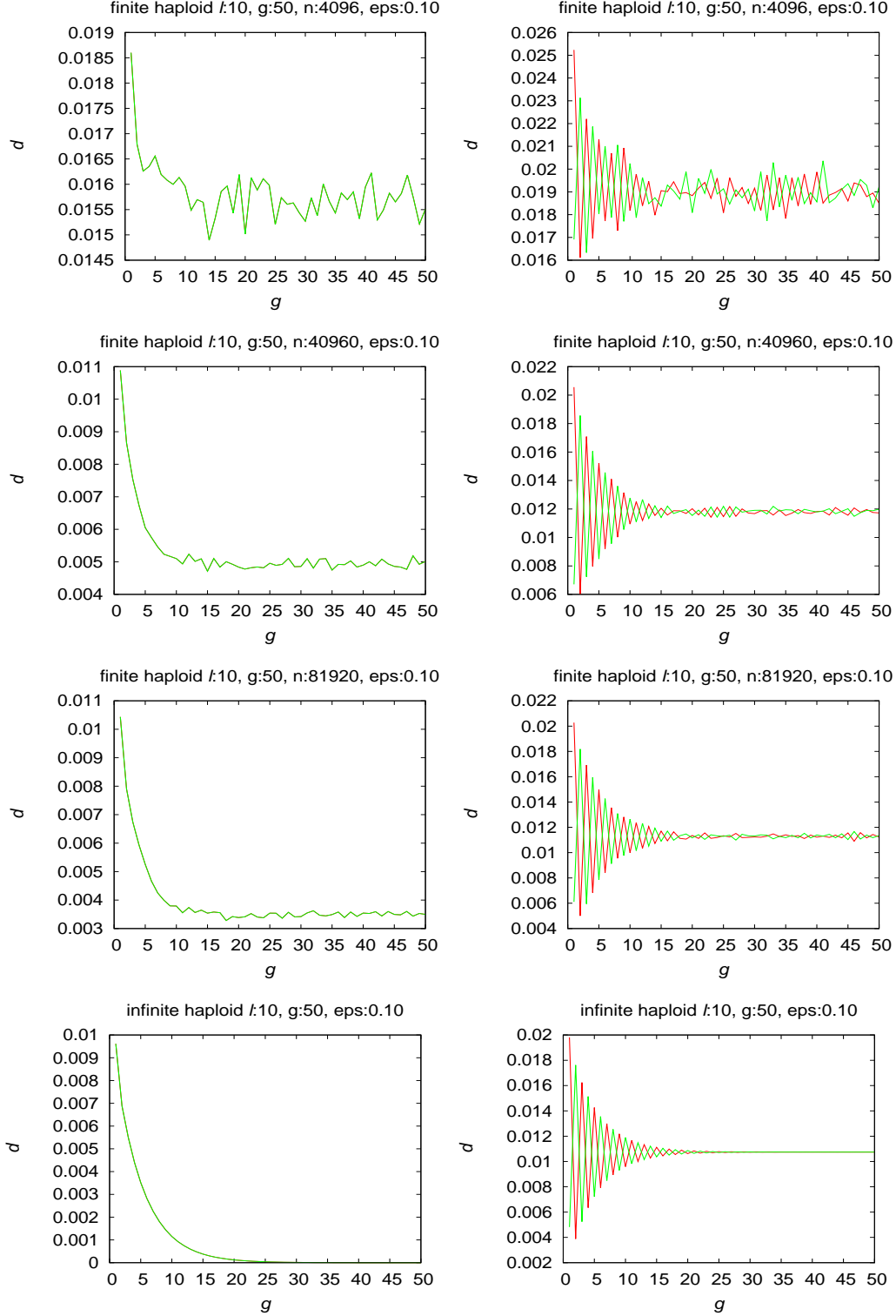
**Figure 3.15: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 8$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



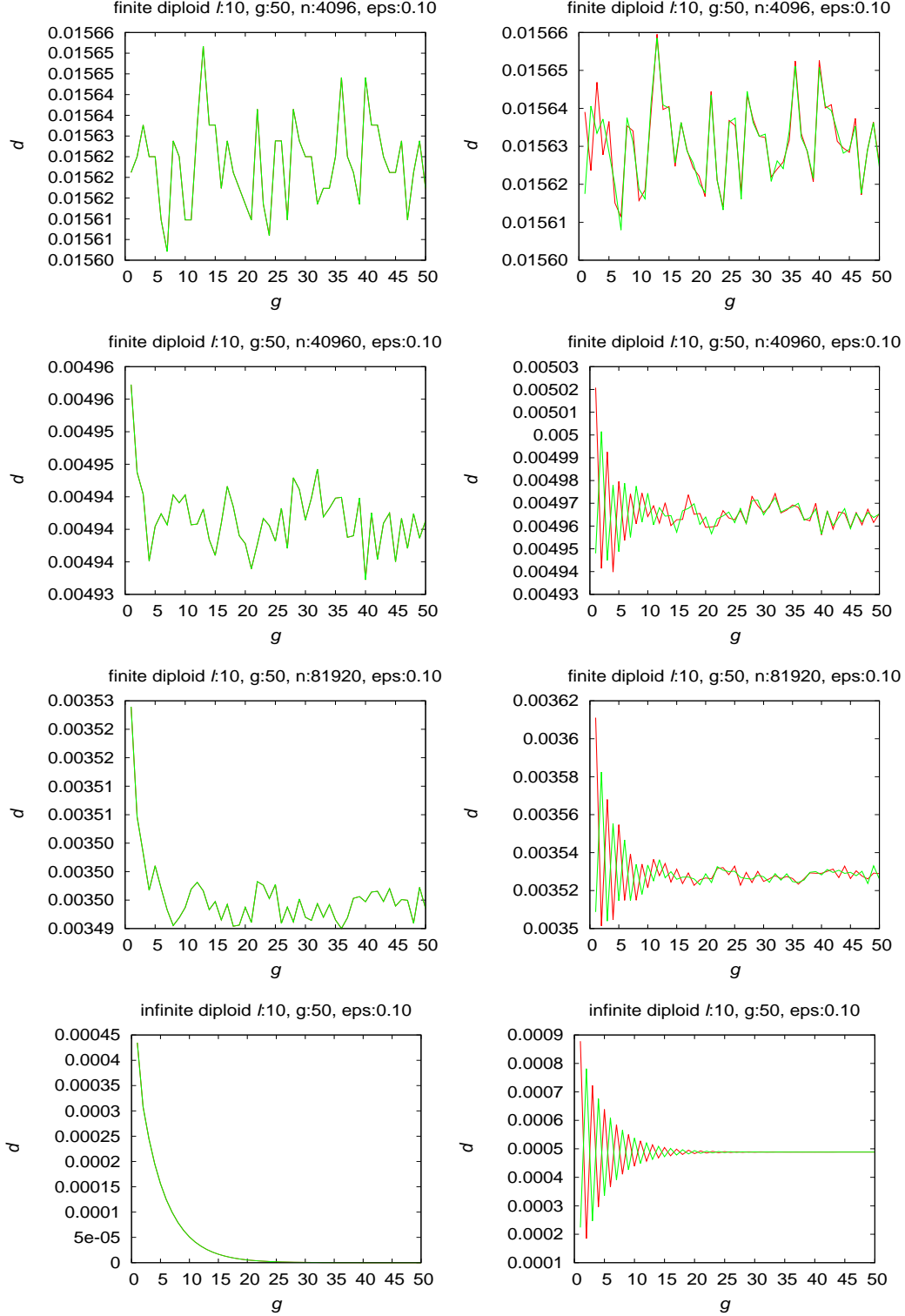
**Figure 3.16: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 10$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



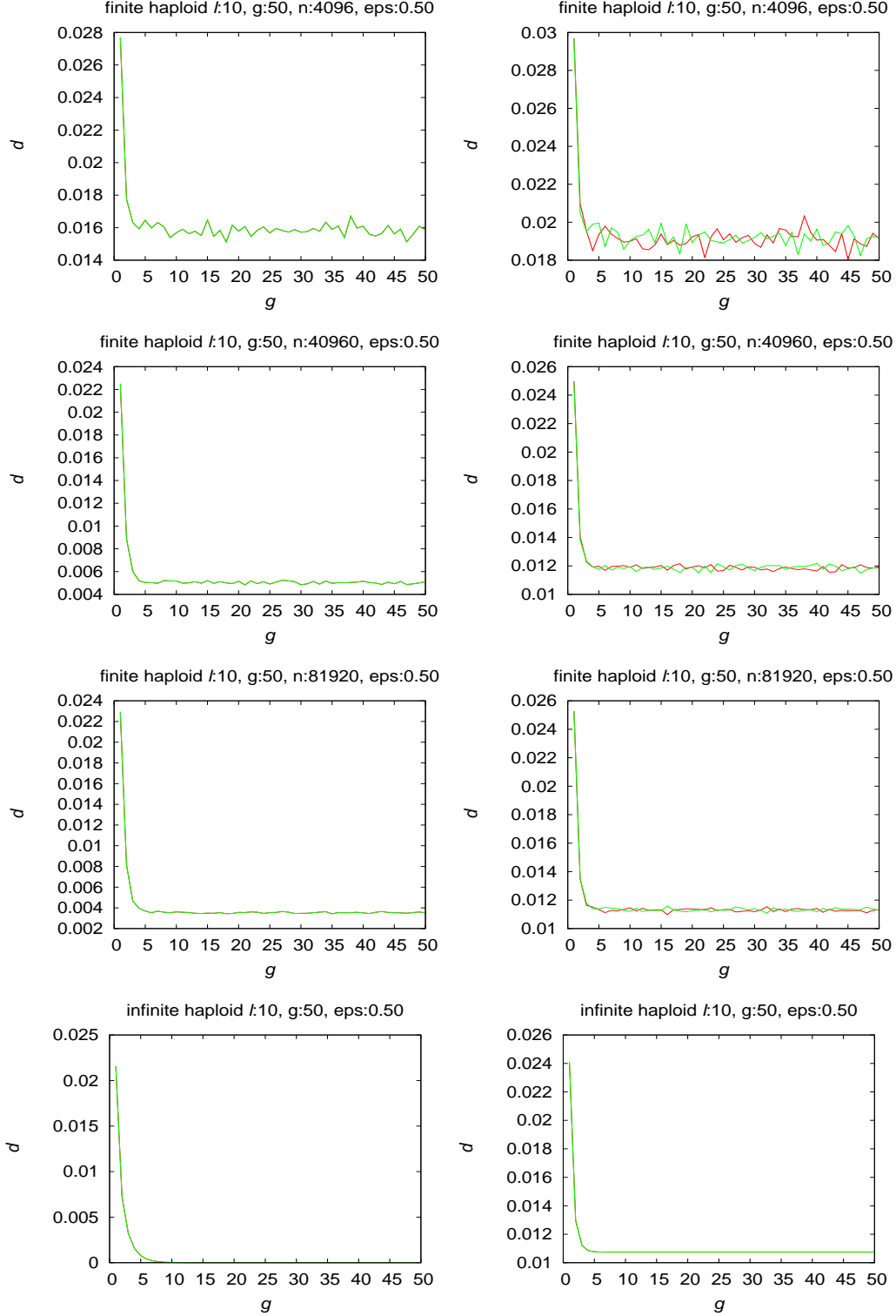
**Figure 3.17: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 10$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



**Figure 3.18: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 10$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

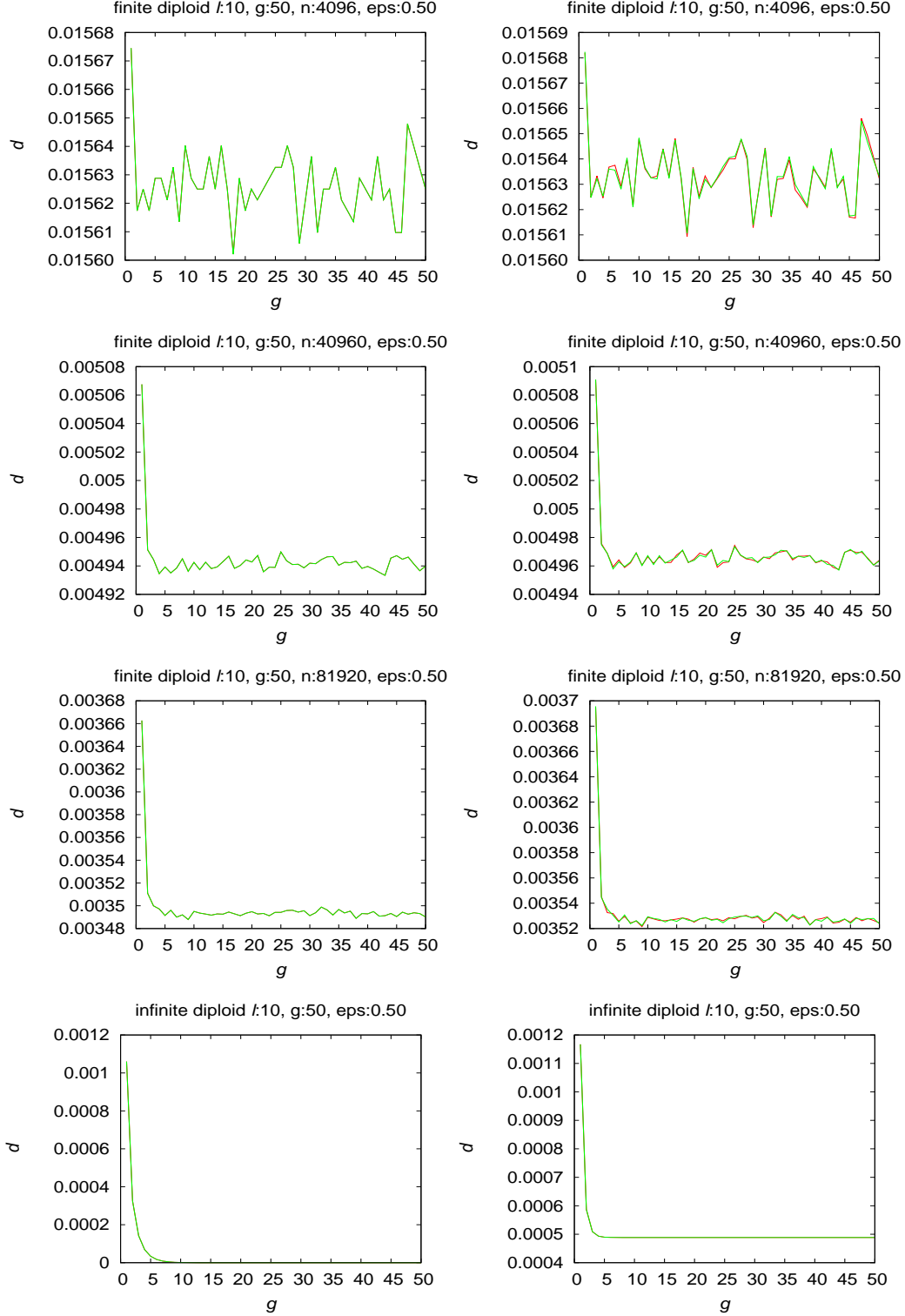


**Figure 3.19: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 10$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

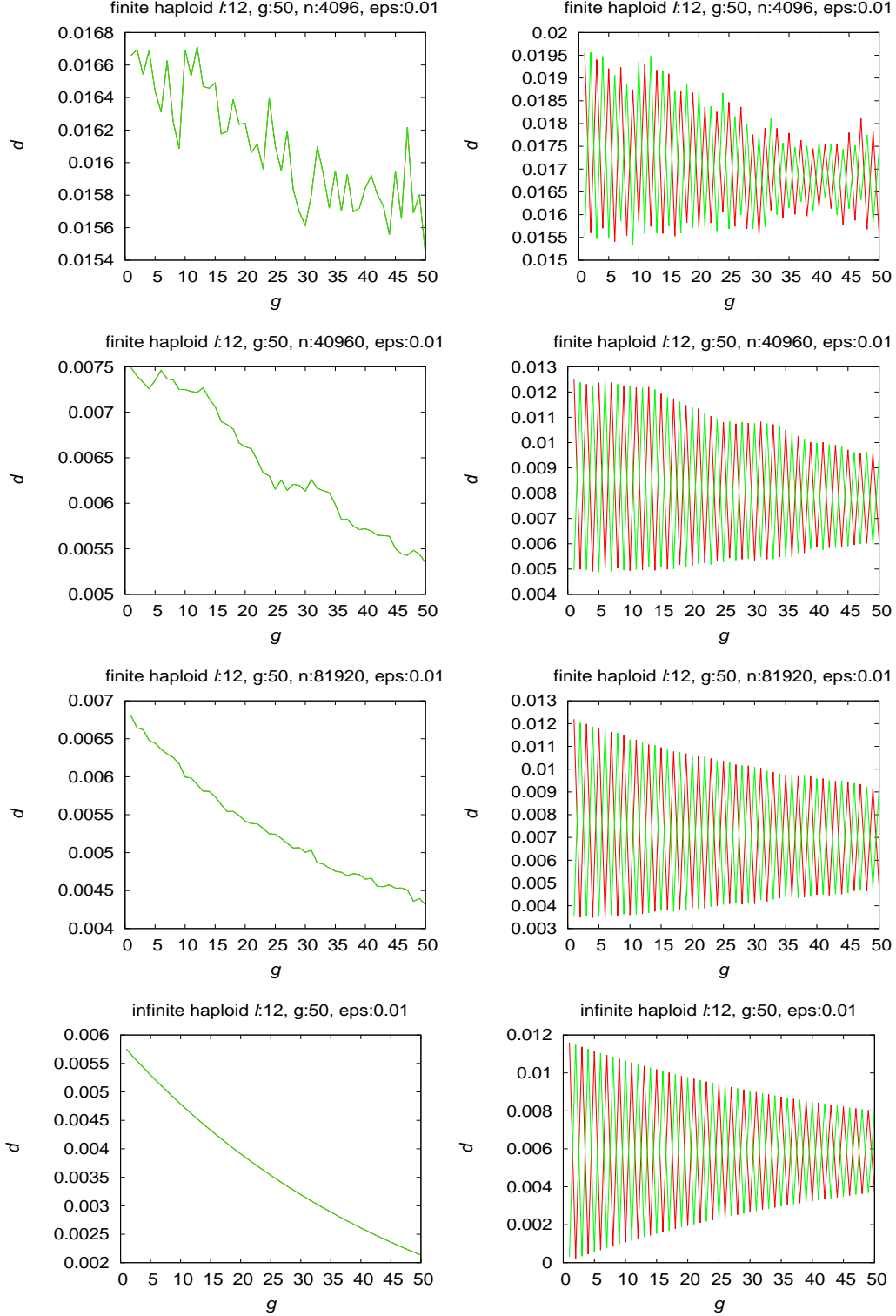


**Figure 3.20: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 10$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

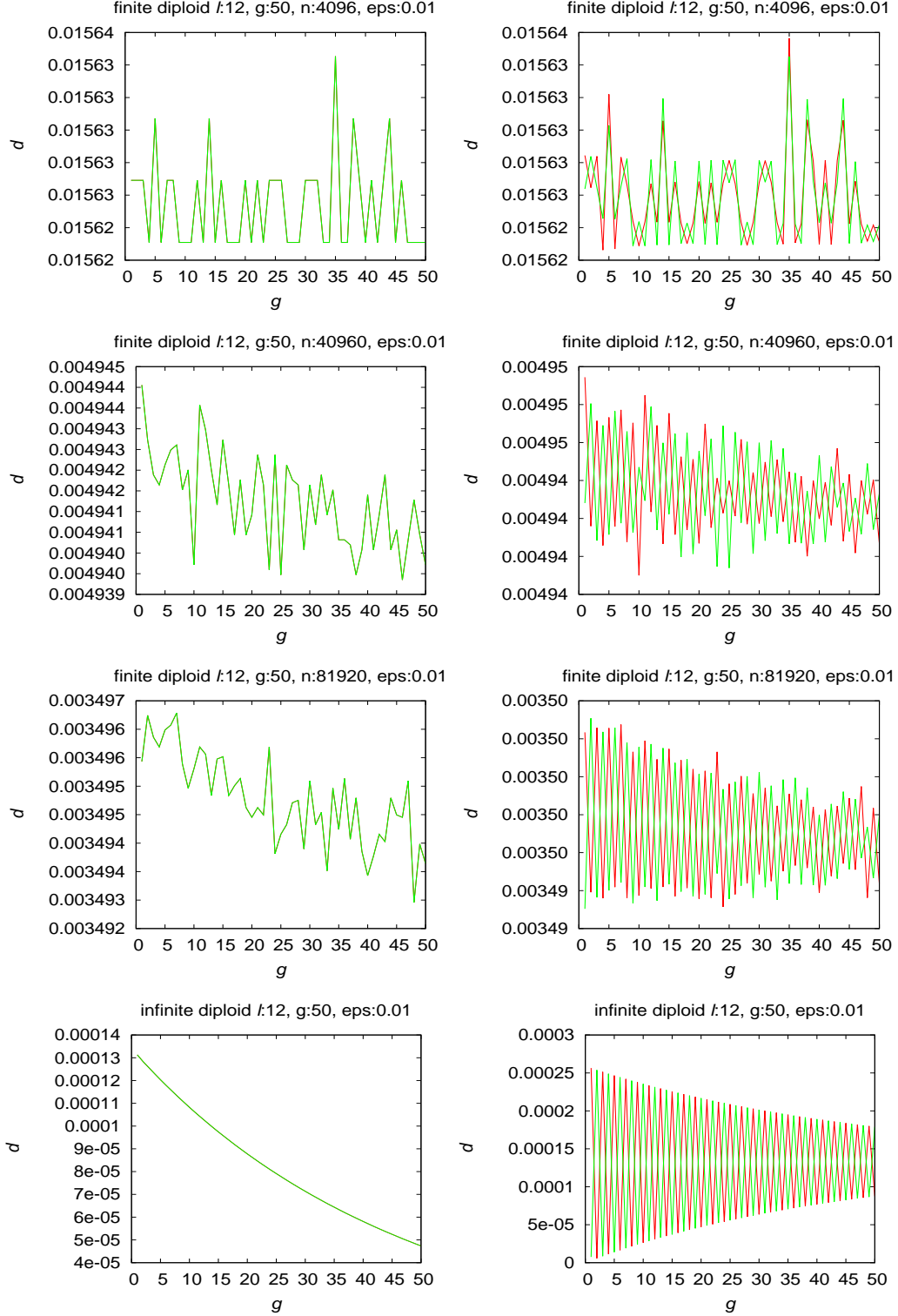




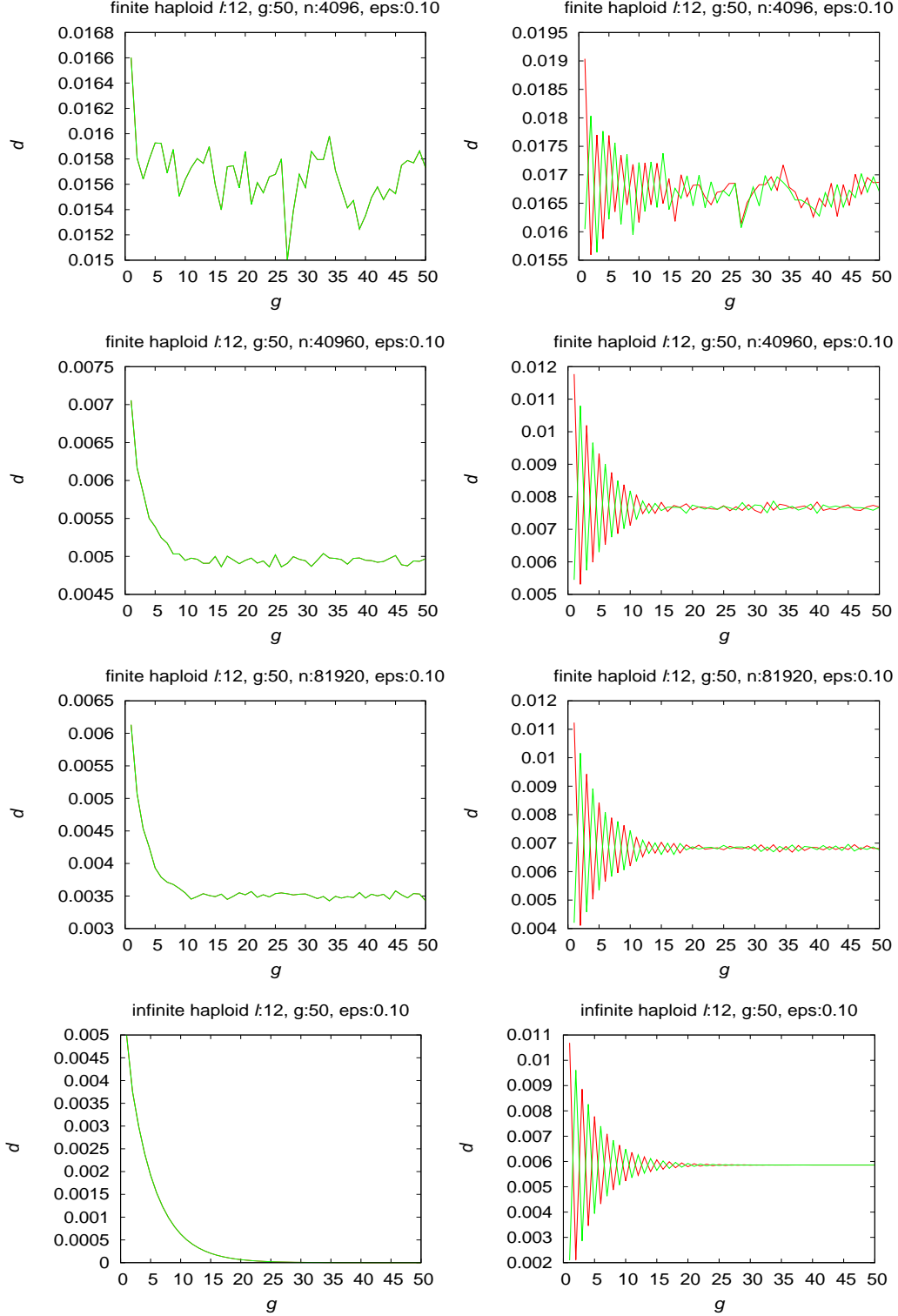
**Figure 3.21: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 10$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



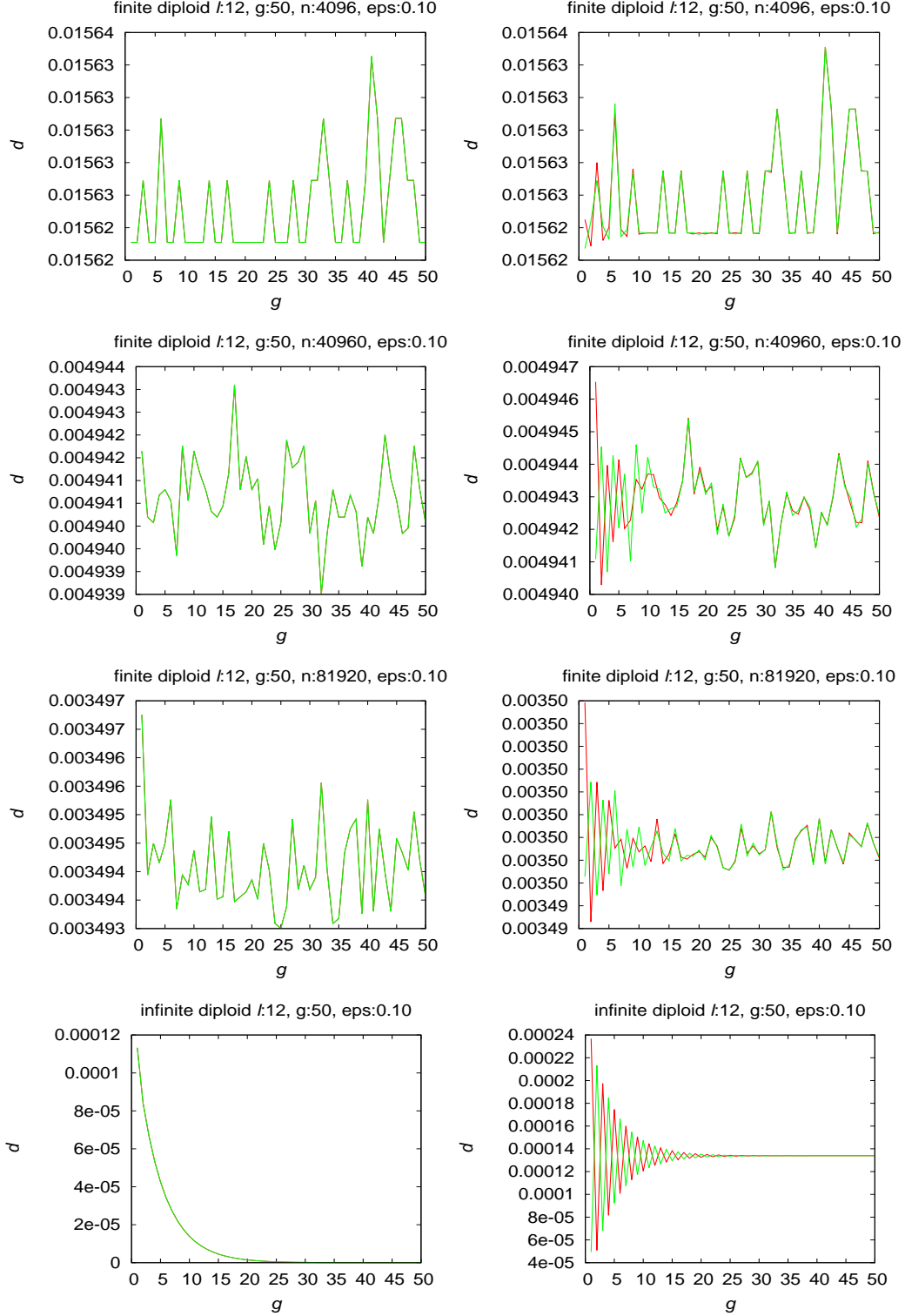
**Figure 3.22: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 12$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



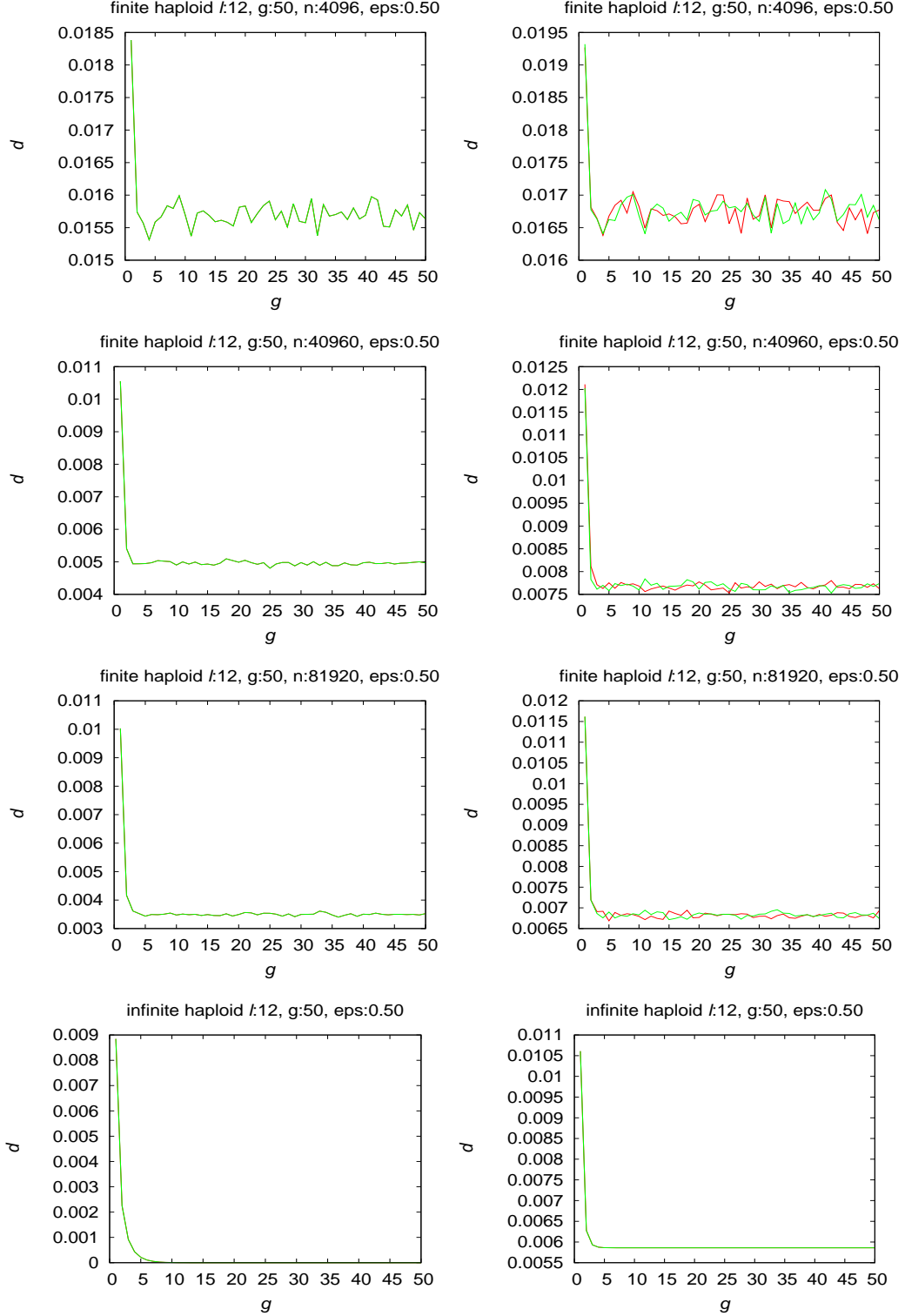
**Figure 3.23: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 12$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



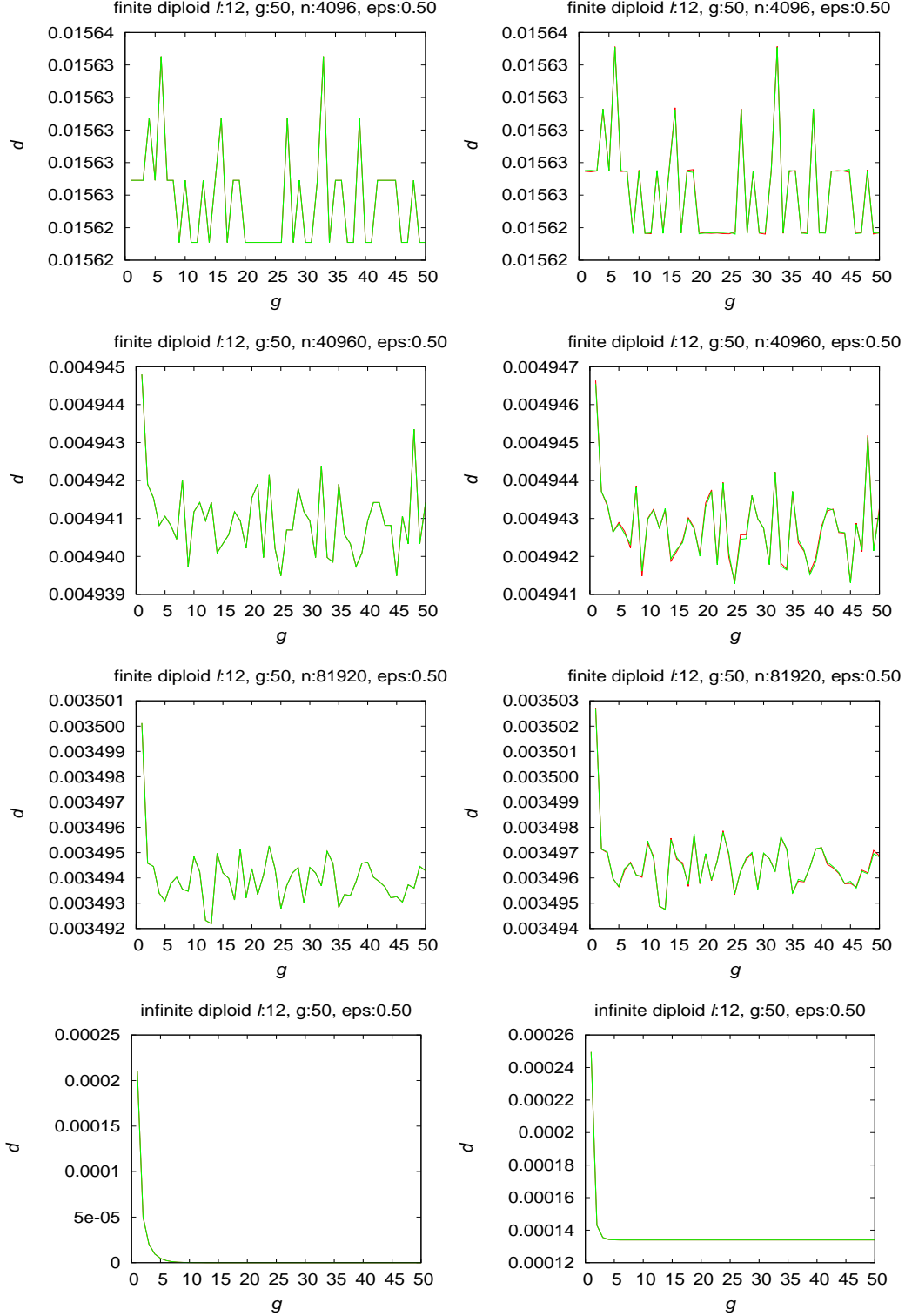
**Figure 3.24: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 12$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



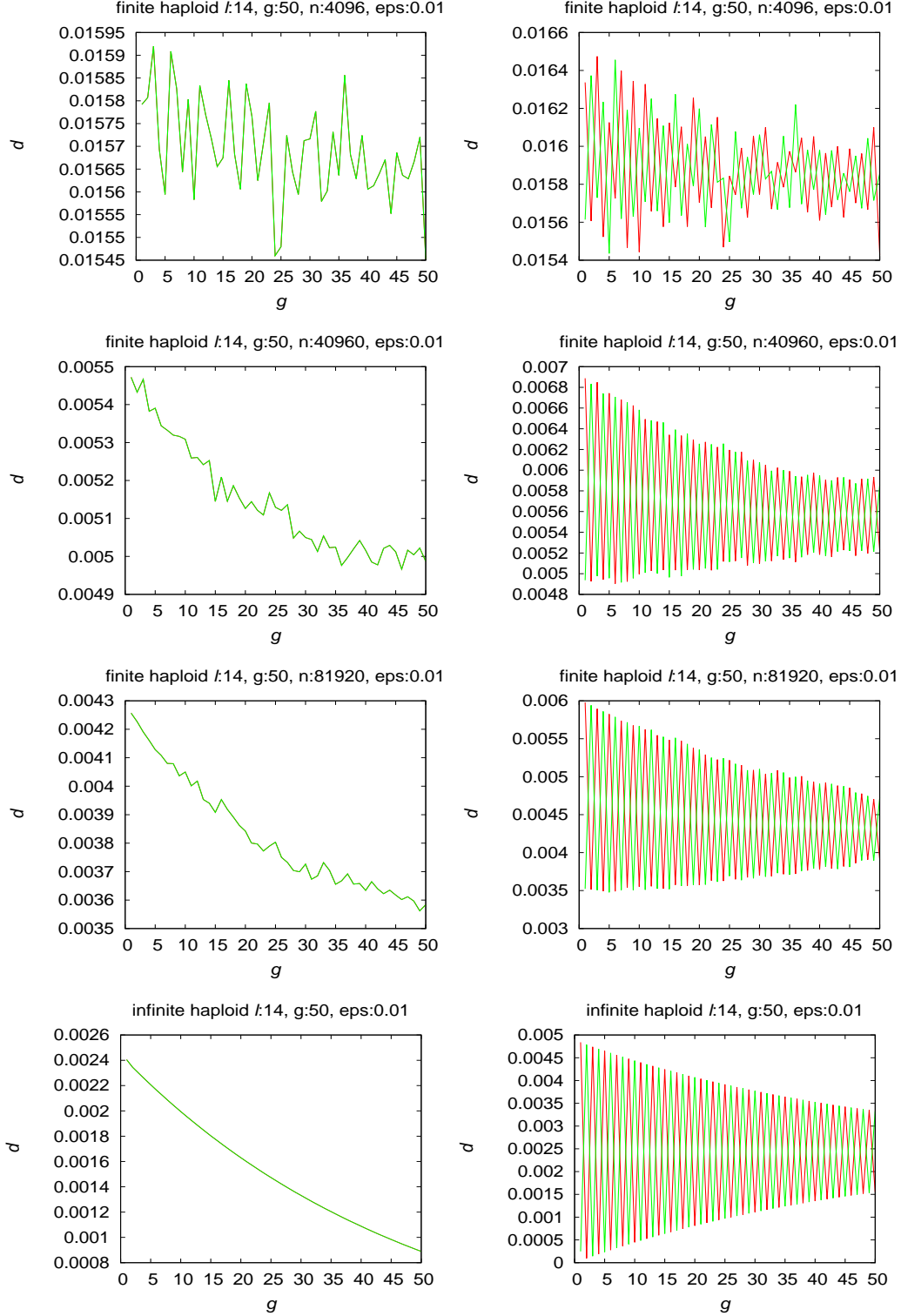
**Figure 3.25: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 12$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



**Figure 3.26: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 12$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

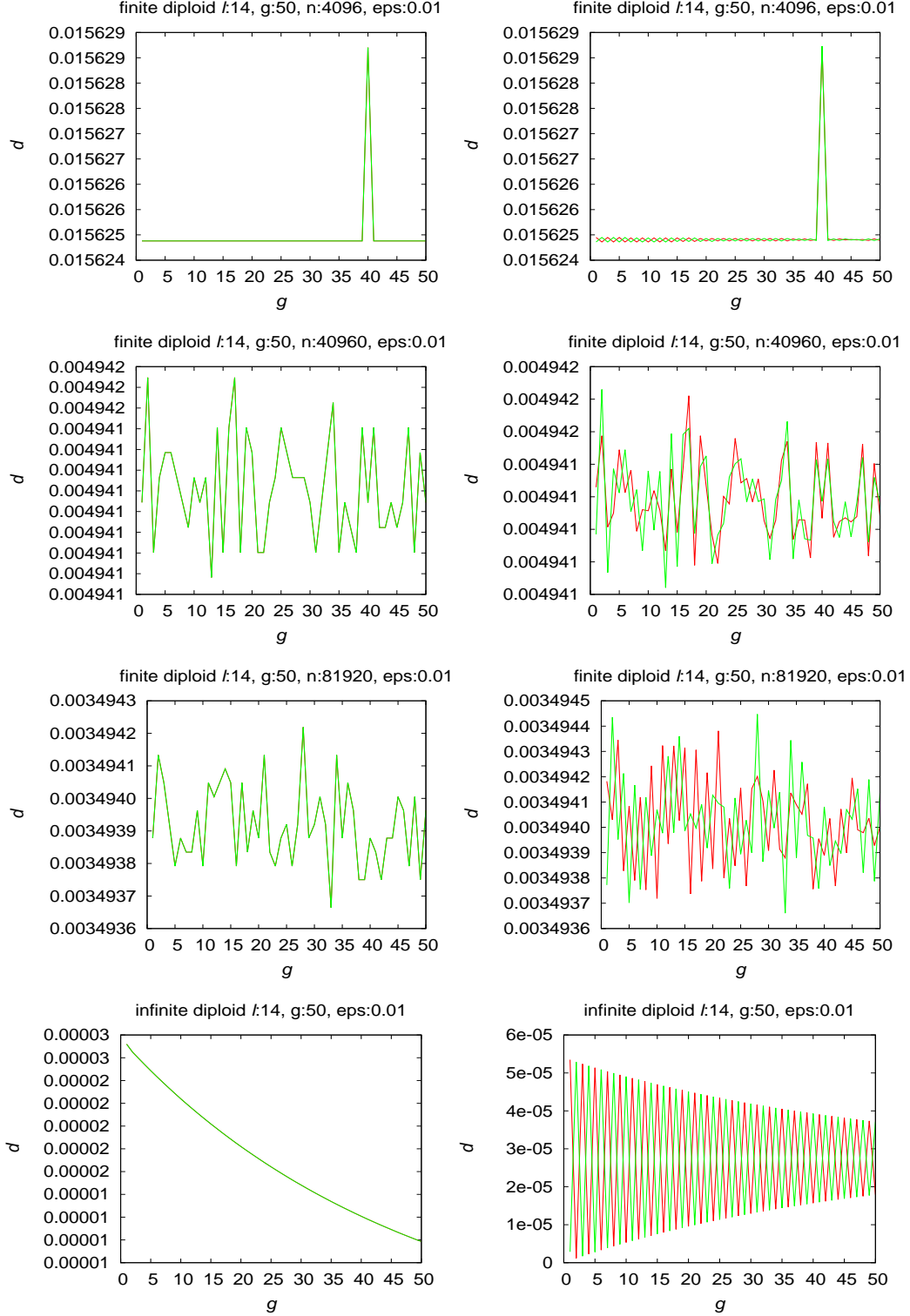


**Figure 3.27: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 12$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

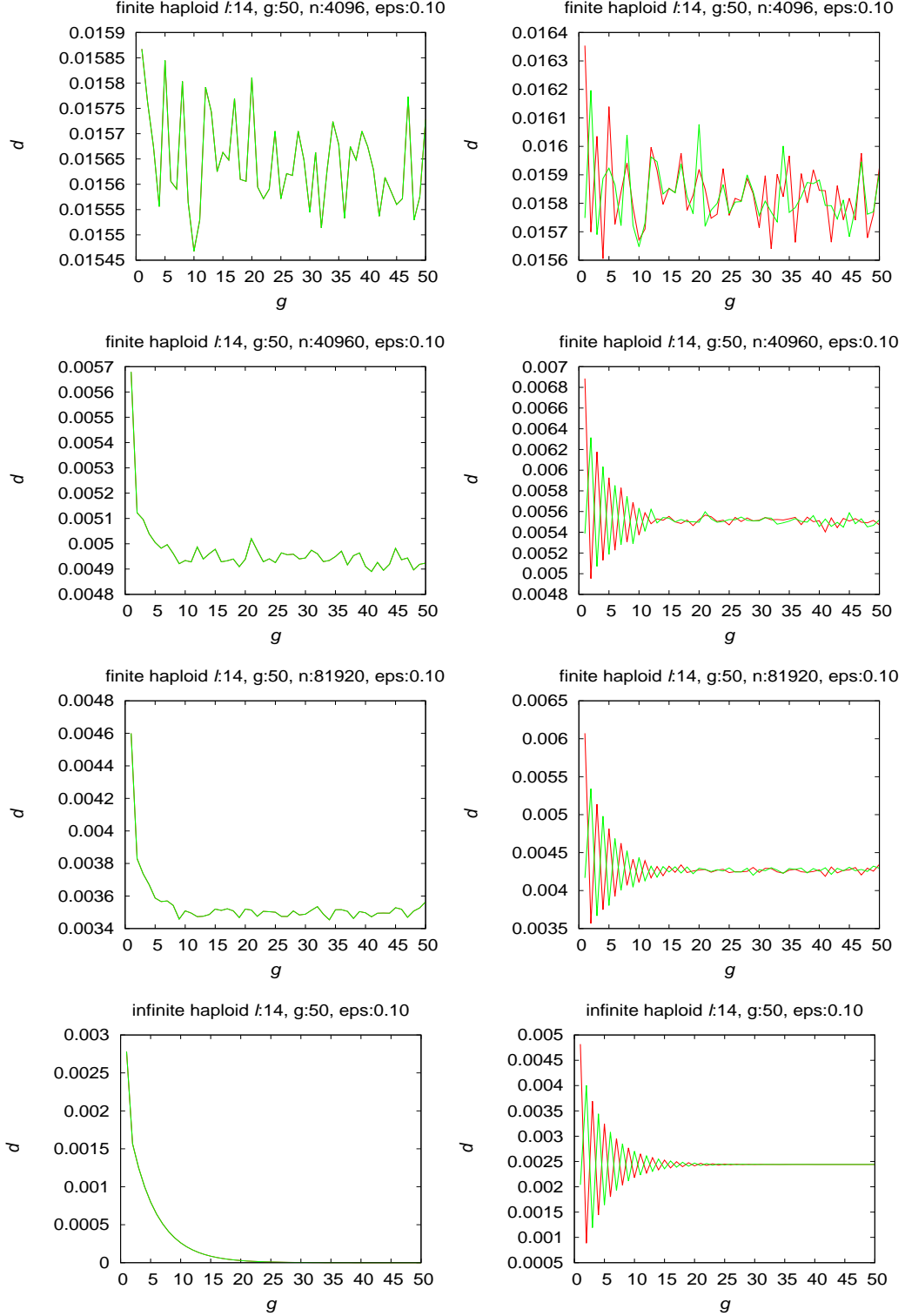


**Figure 3.28: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 14$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

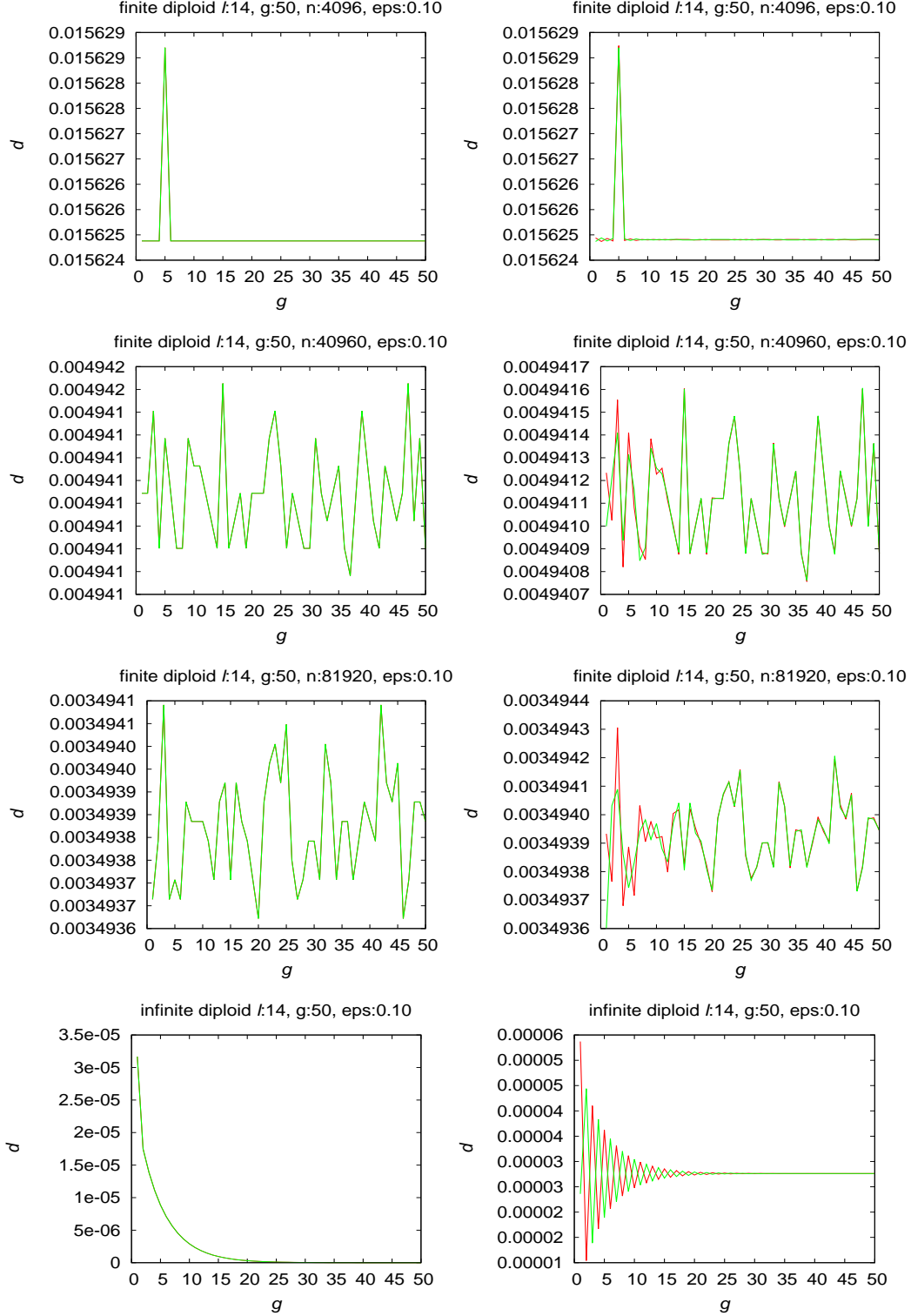




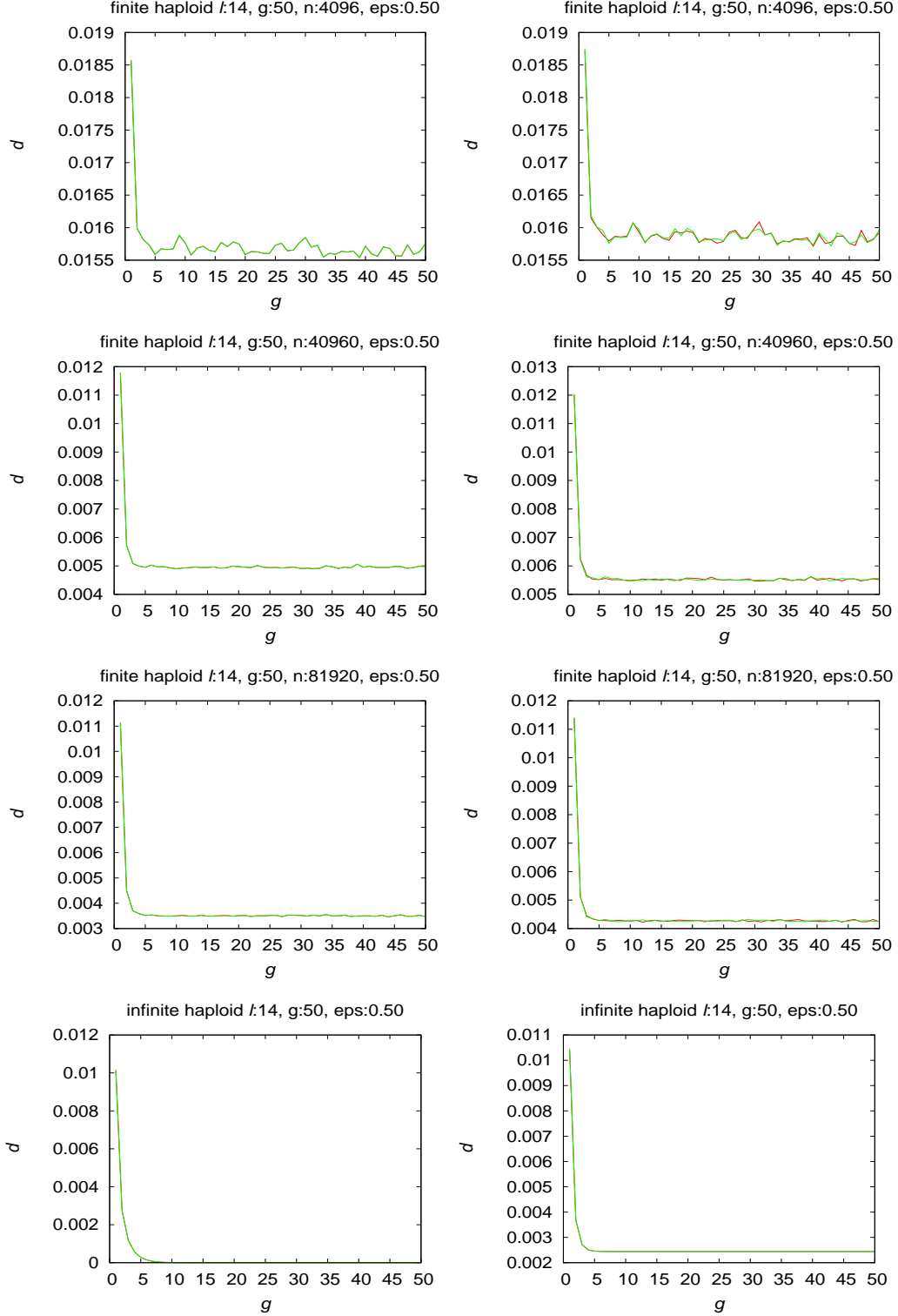
**Figure 3.29: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 14$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



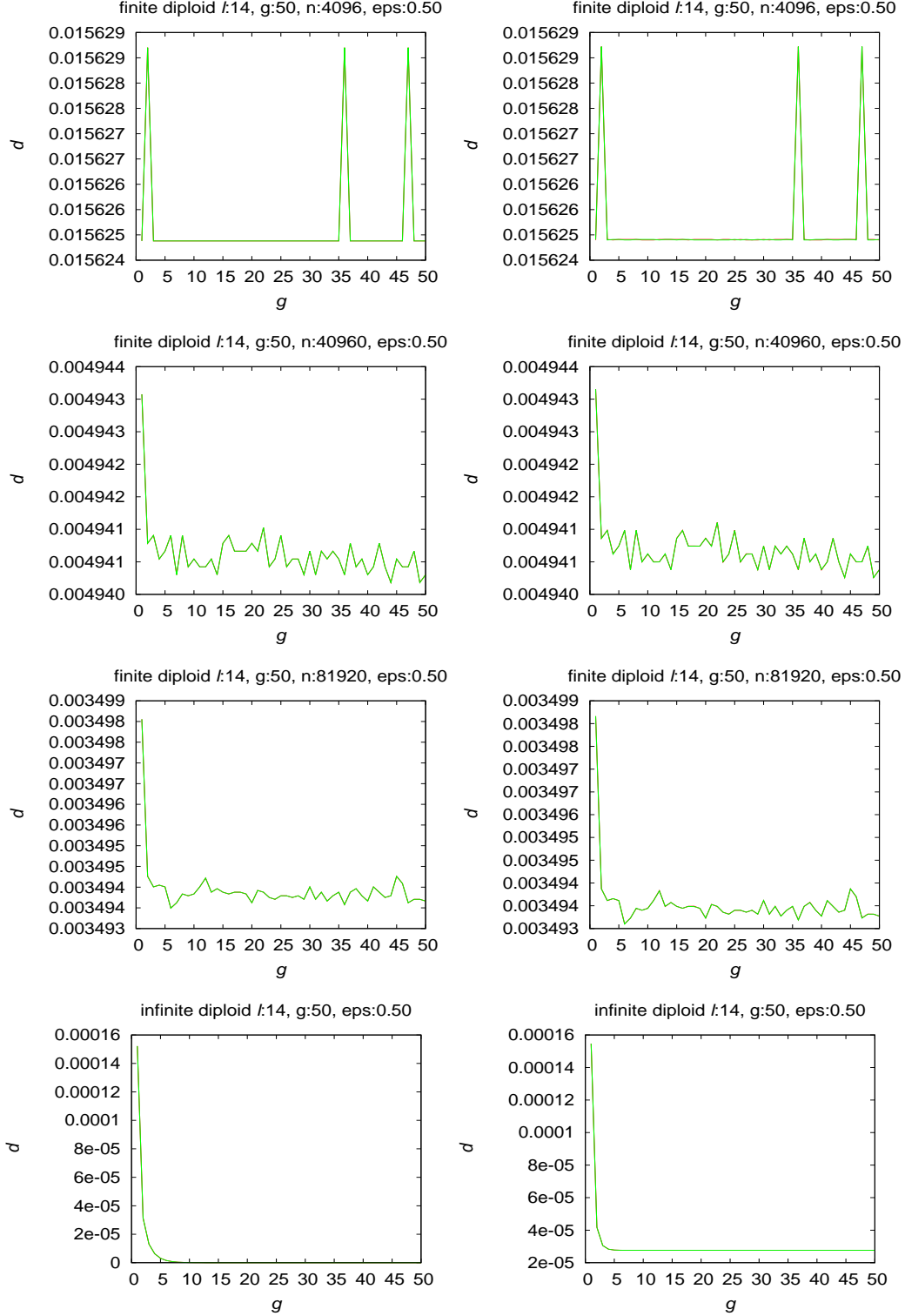
**Figure 3.30: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 14$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



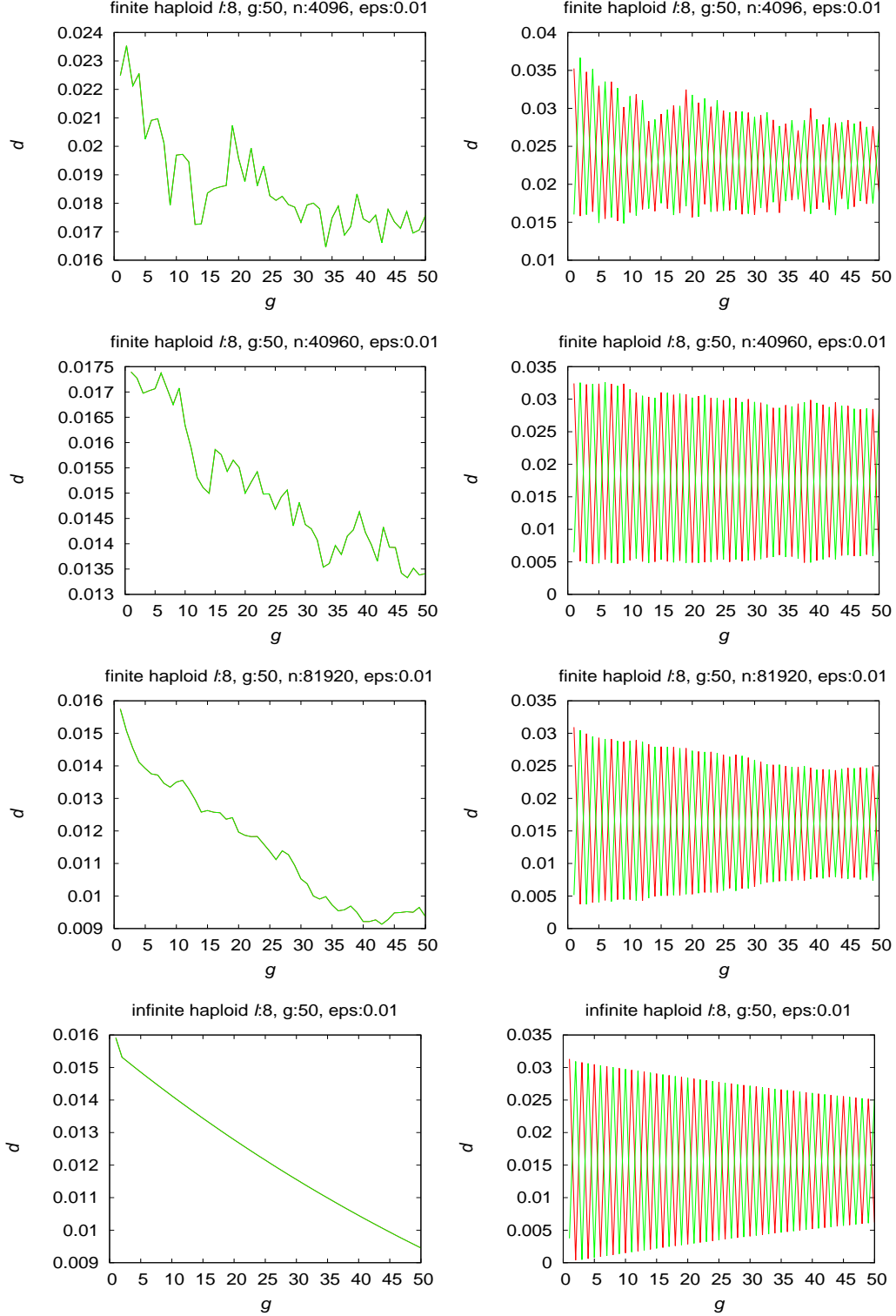
**Figure 3.31: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 14$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



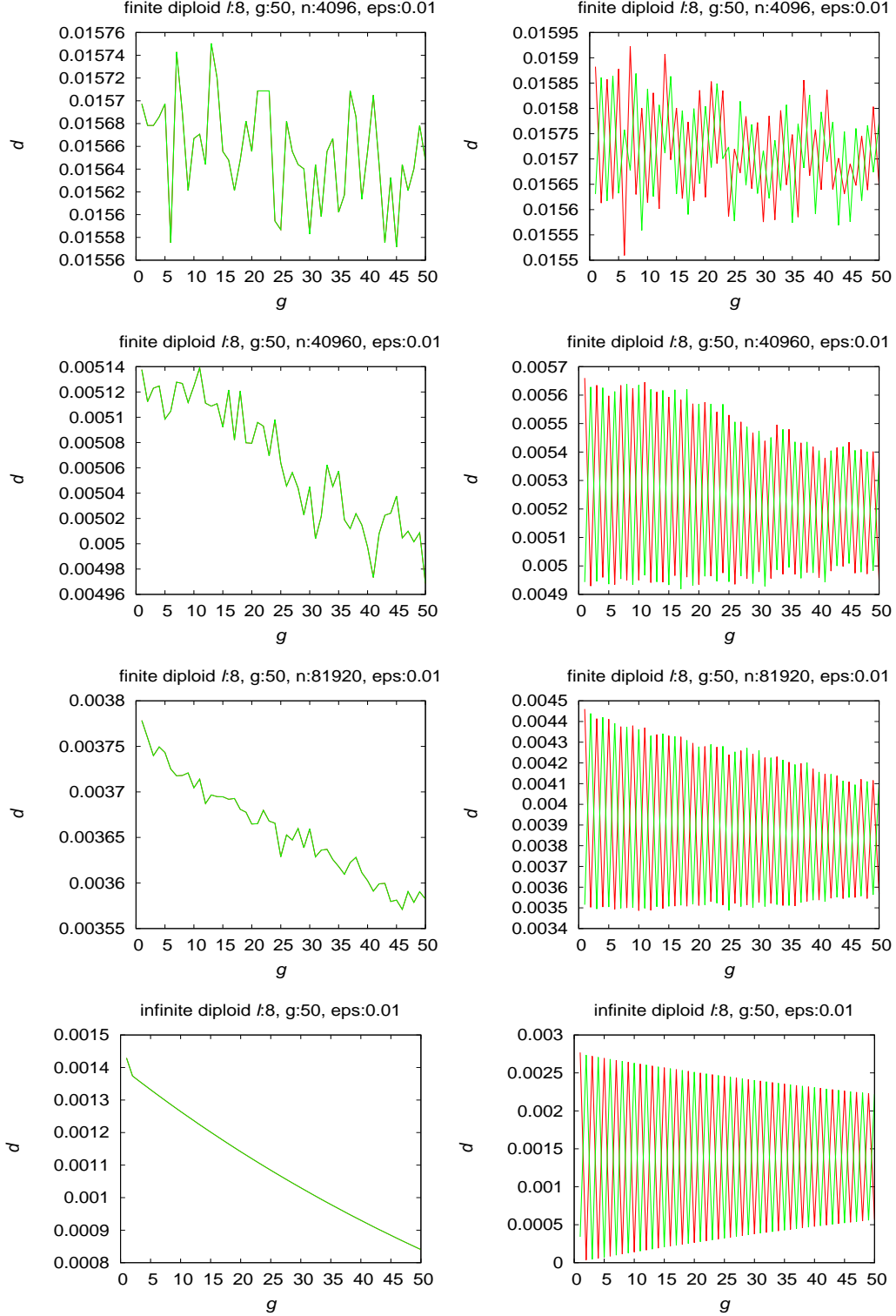
**Figure 3.32: Infinite and finite haploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 14$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



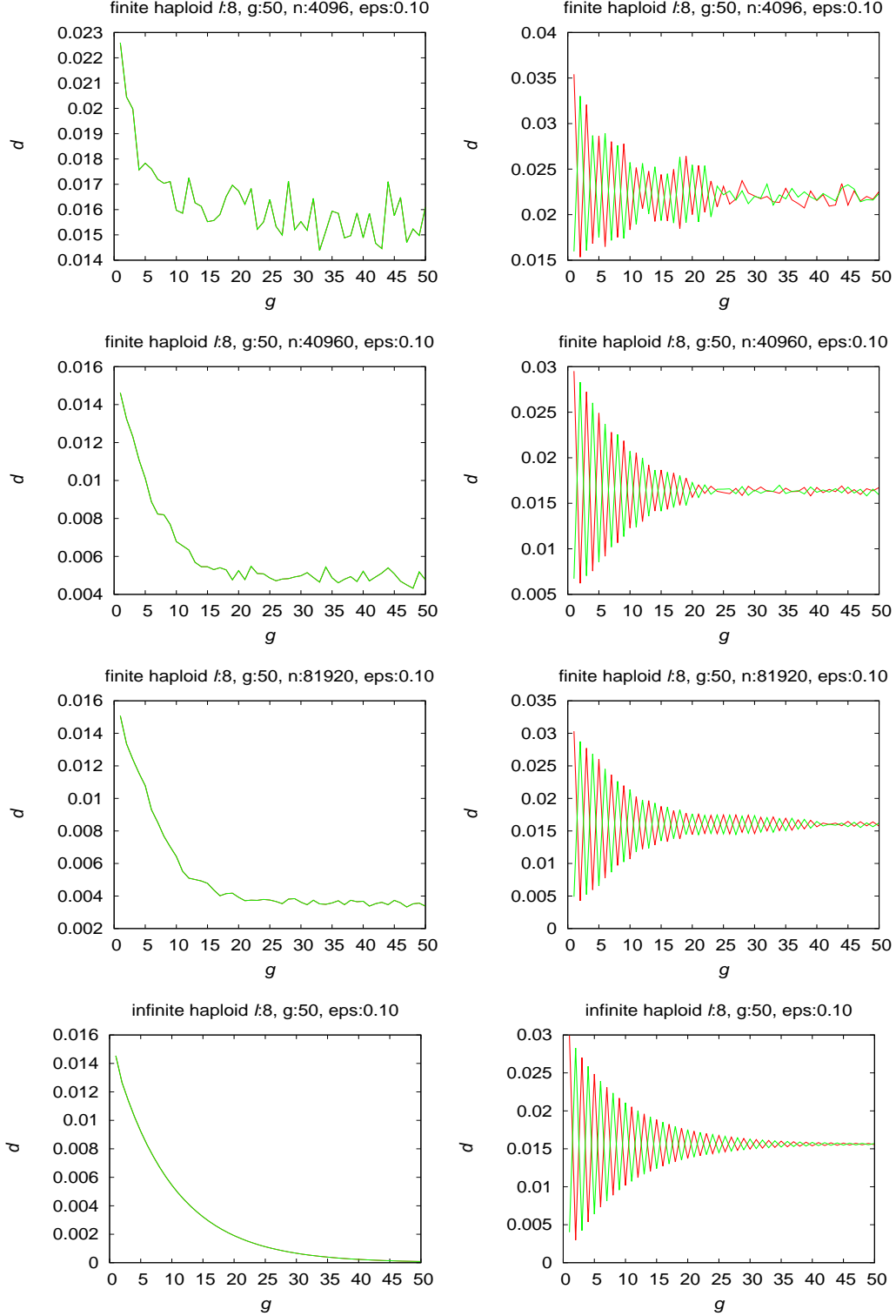
**Figure 3.33: Infinite and finite diploid population oscillation behavior in case of violation in  $\mu$  for genome length  $\ell = 14$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



**Figure 3.34: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 8$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

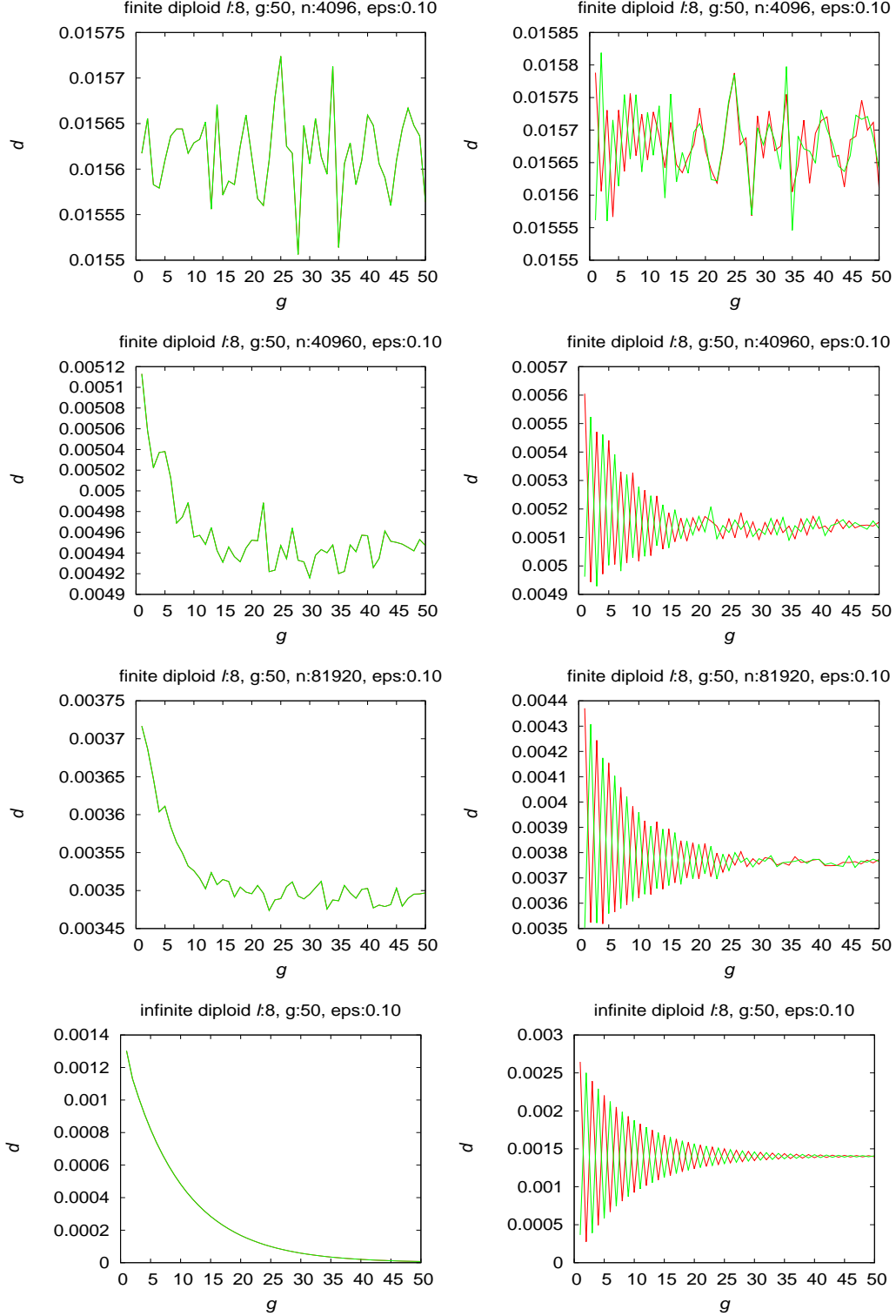


**Figure 3.35: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 8$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

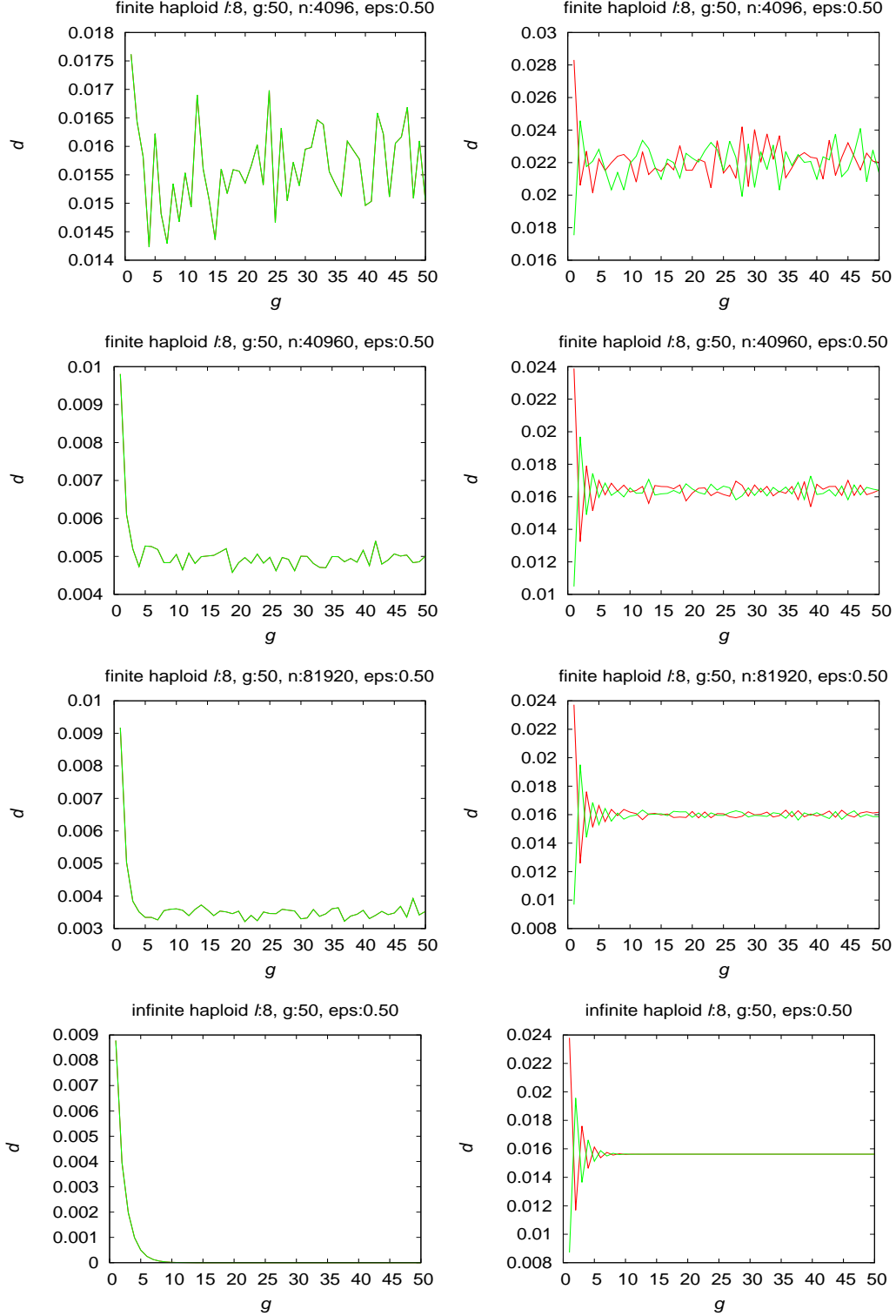


**Figure 3.36: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 8$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

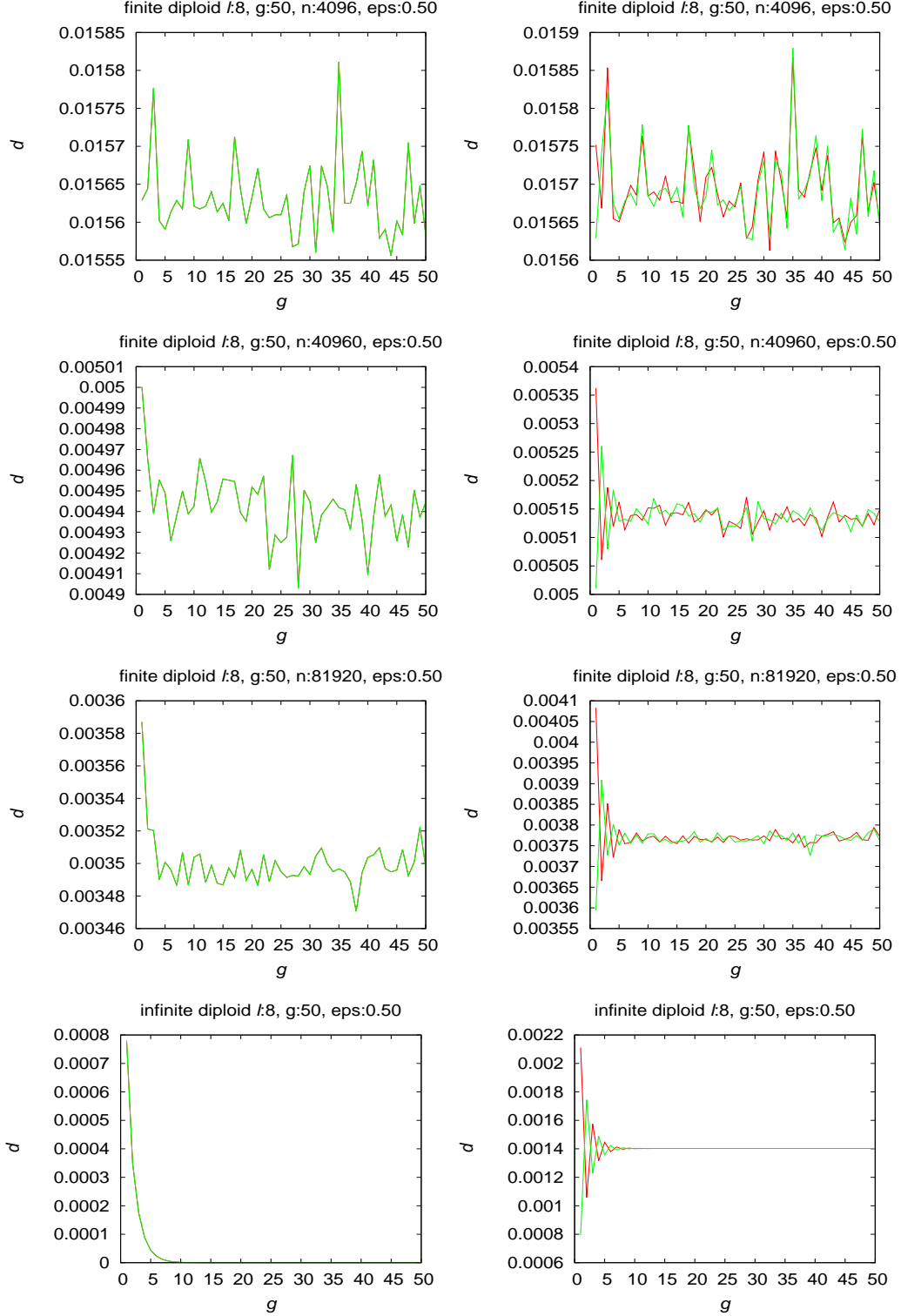




**Figure 3.37: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 8$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



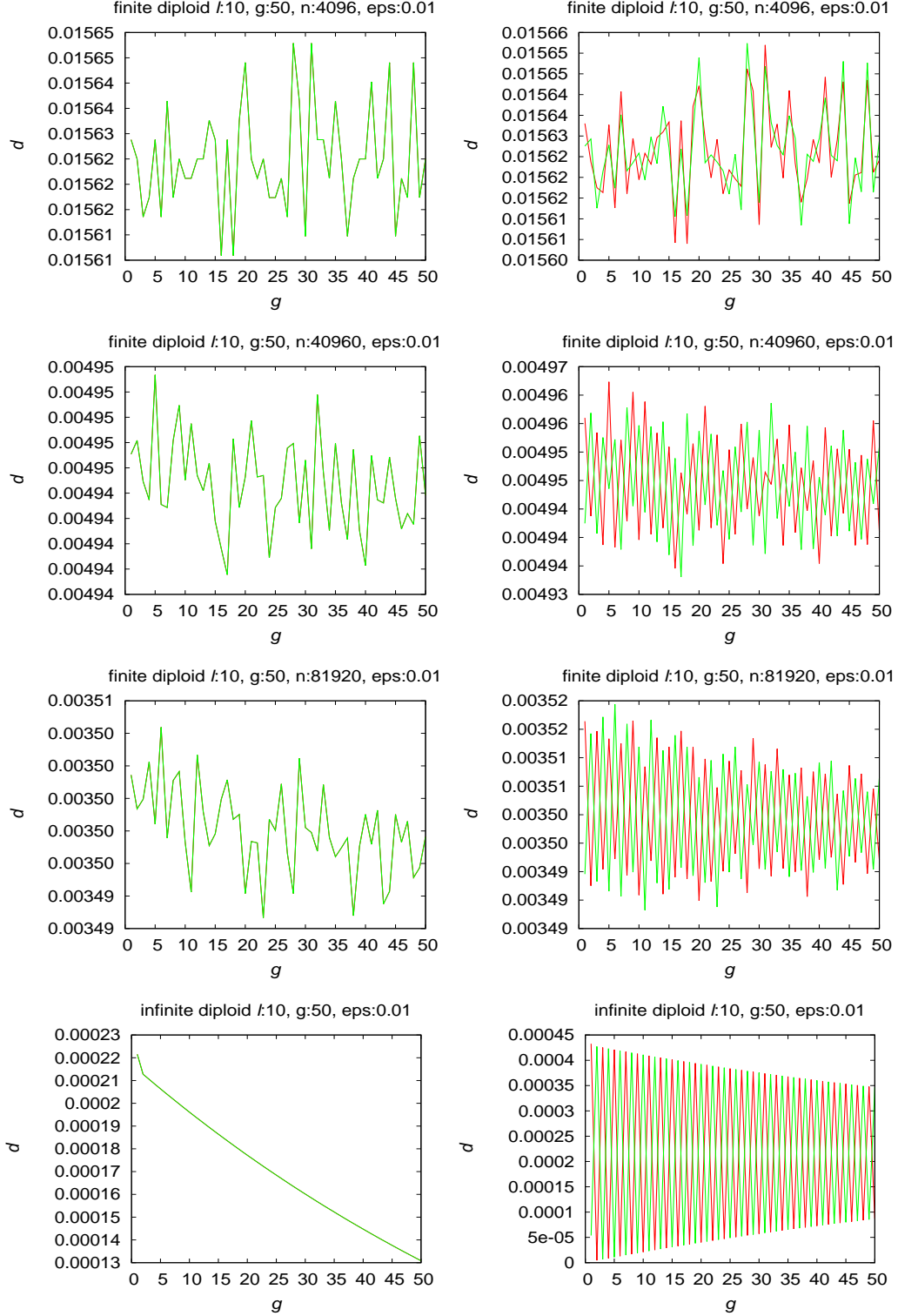
**Figure 3.38: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 8$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



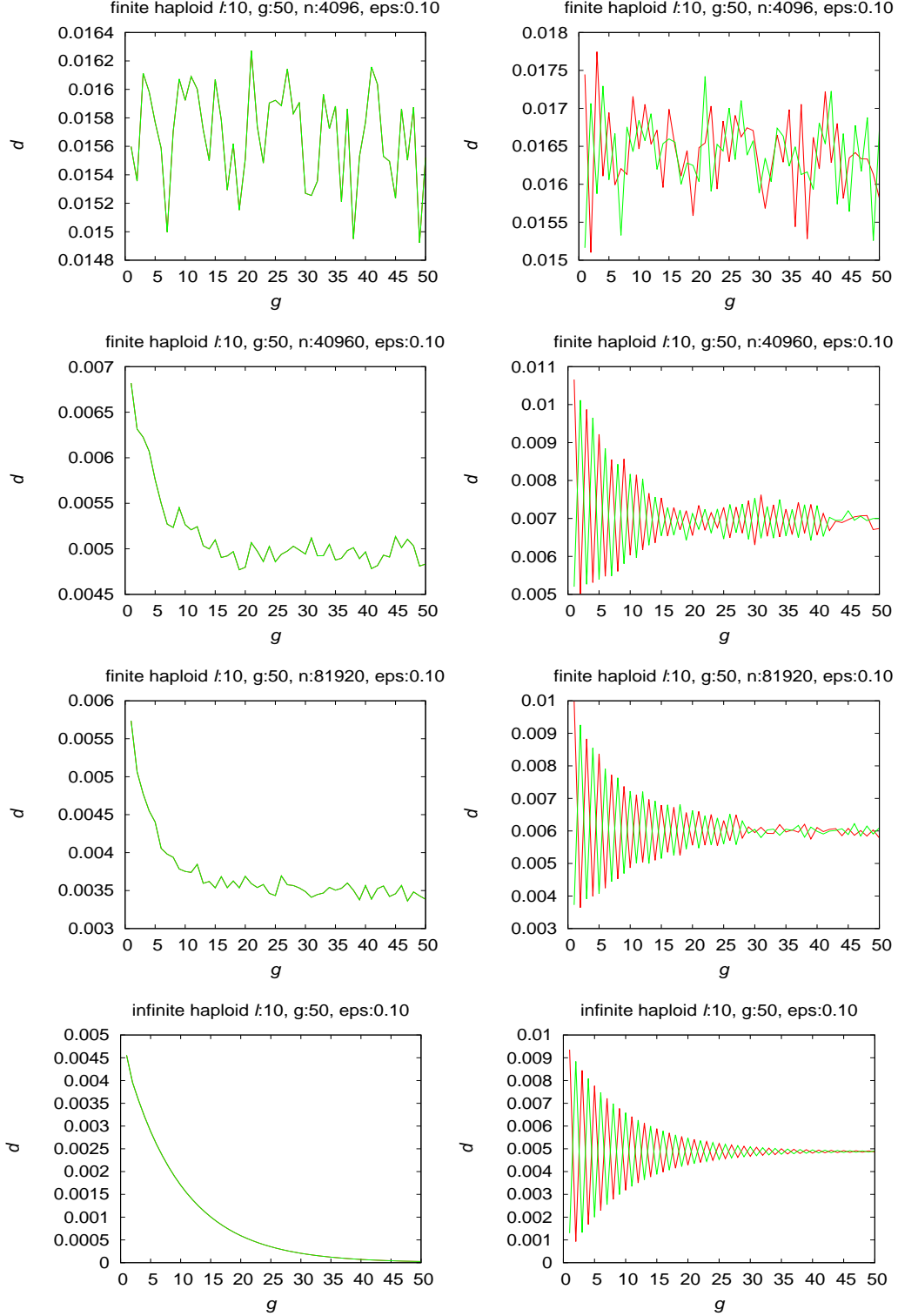
**Figure 3.39: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 8$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



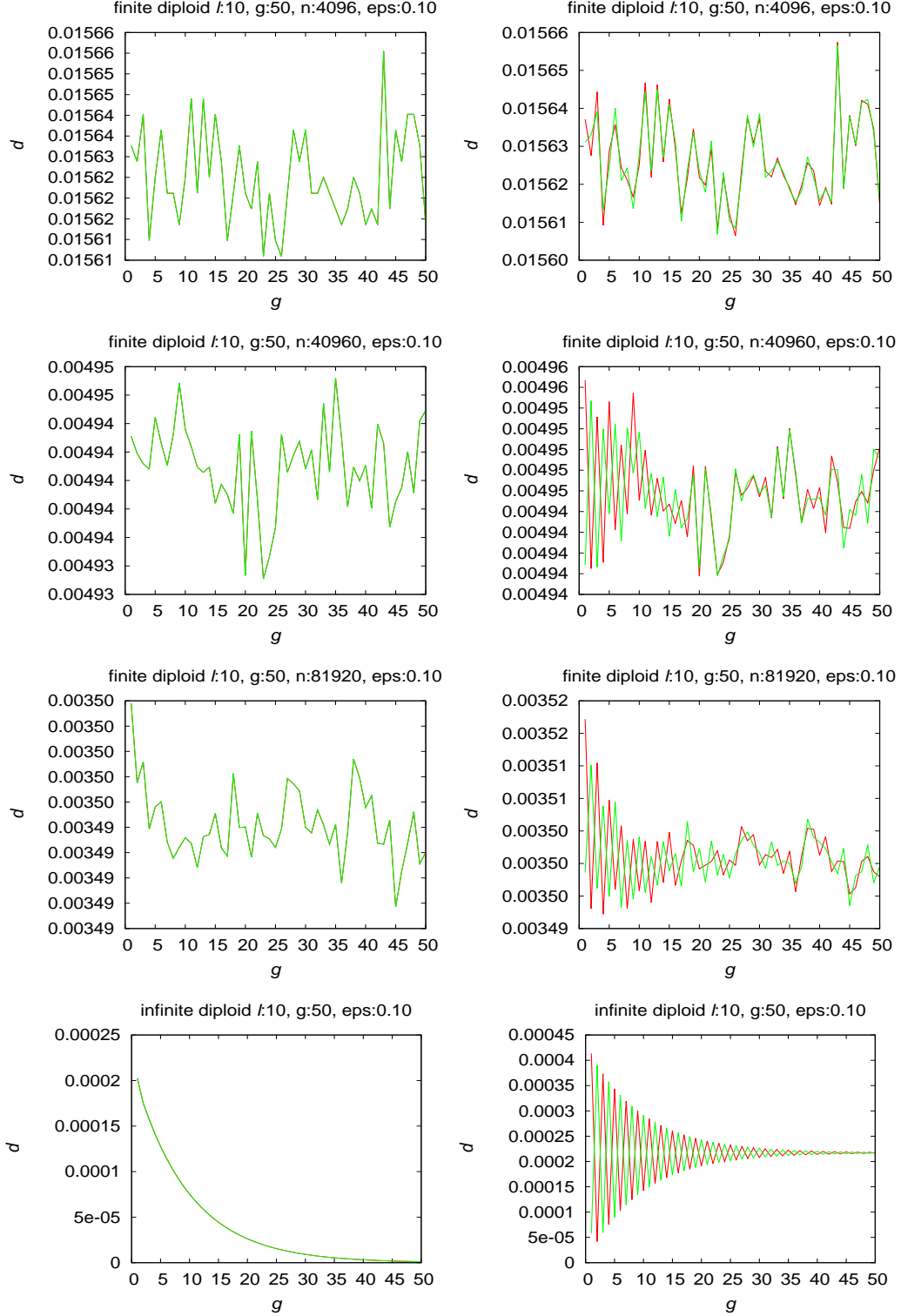
**Figure 3.40: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 10$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



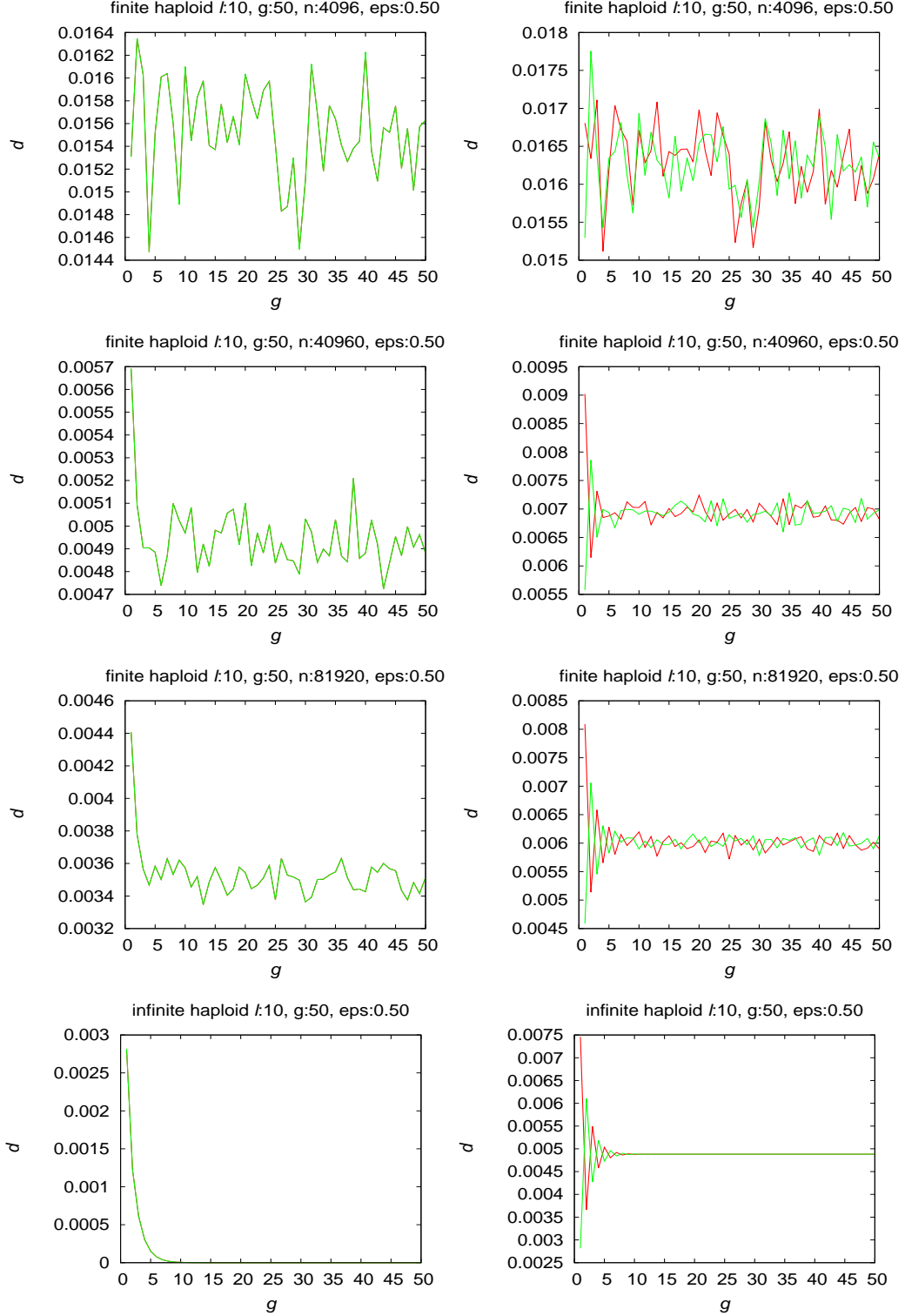
**Figure 3.41: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 10$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



**Figure 3.42: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 10$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

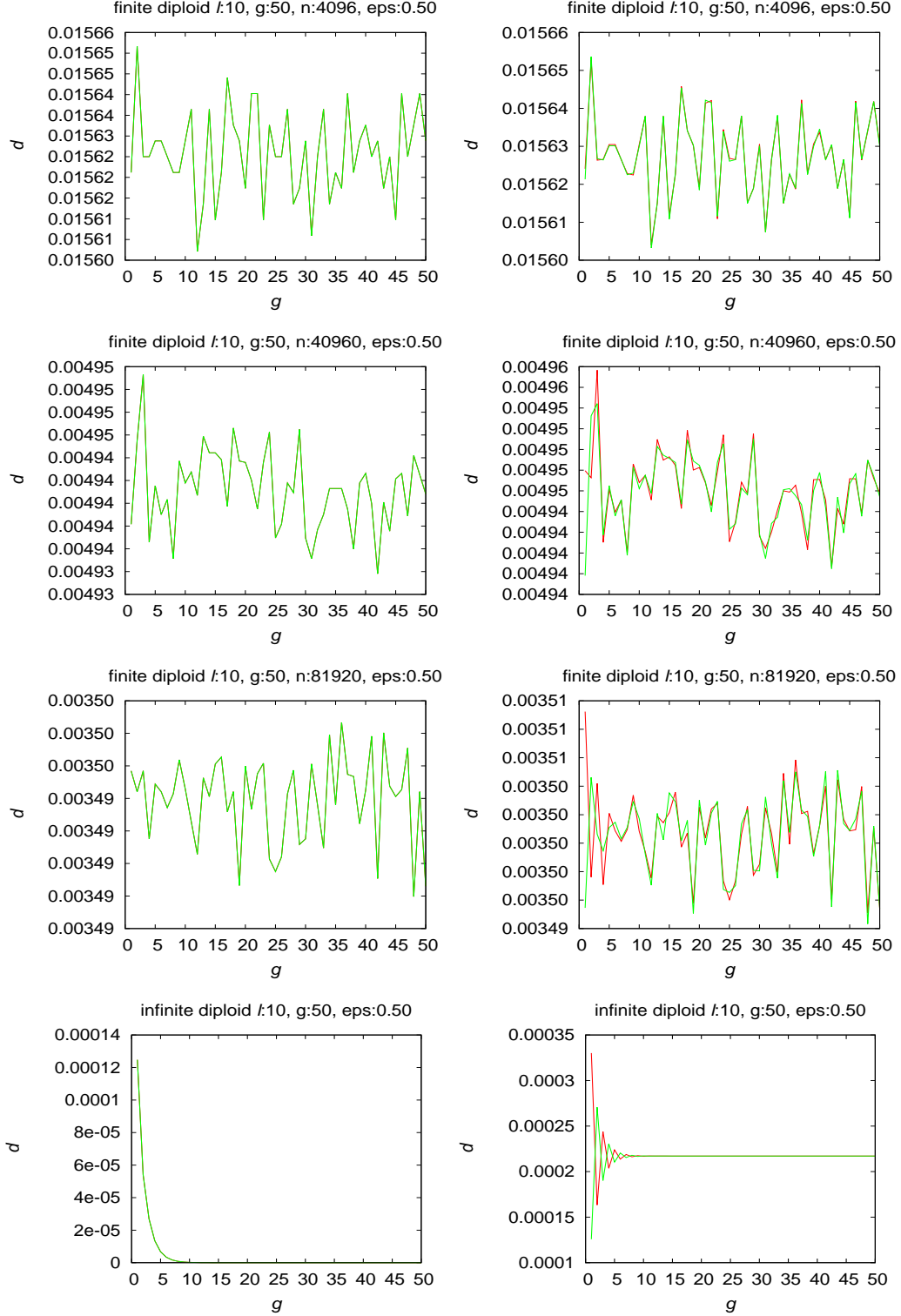


**Figure 3.43: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 10$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

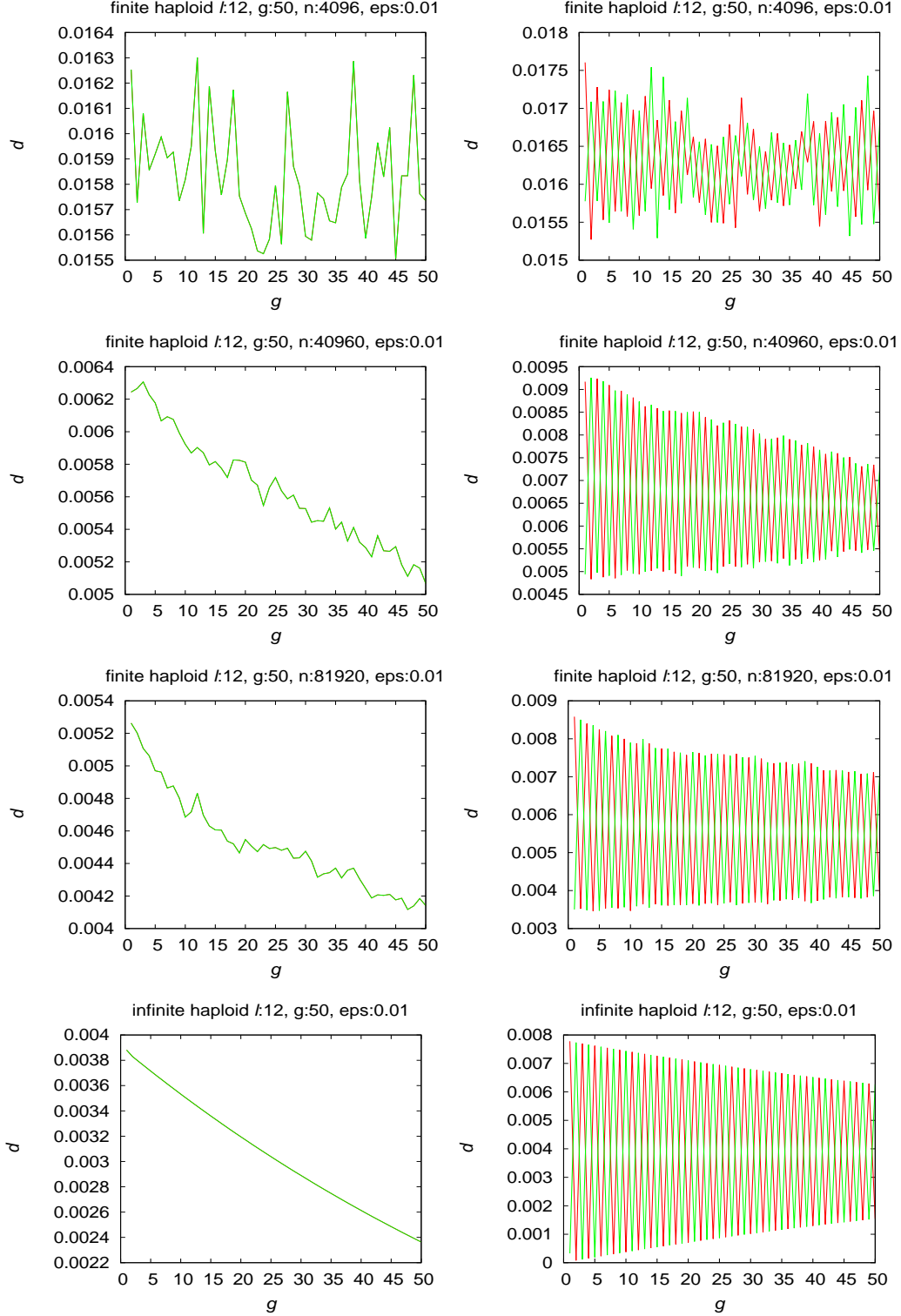


**Figure 3.44: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 10$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

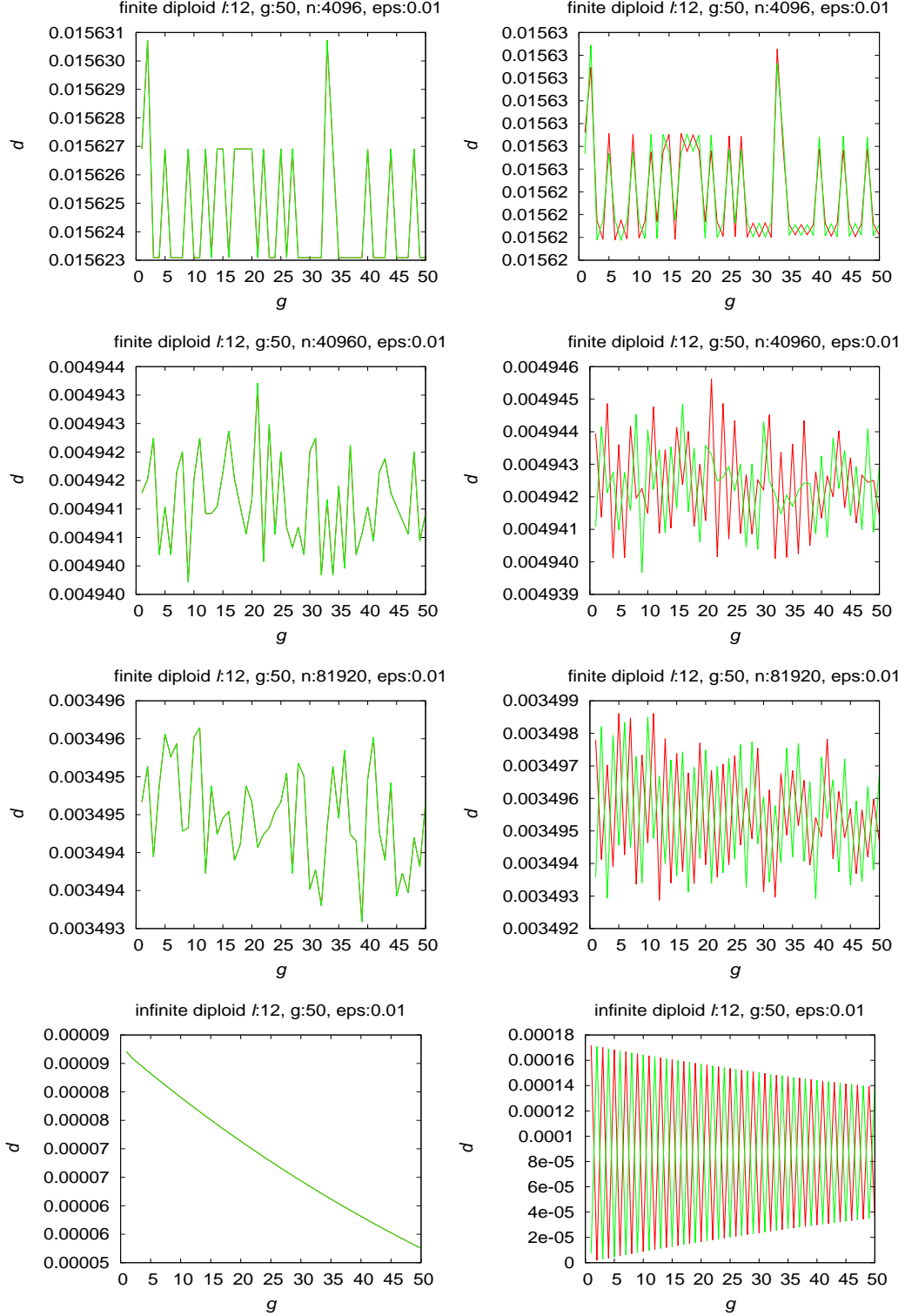




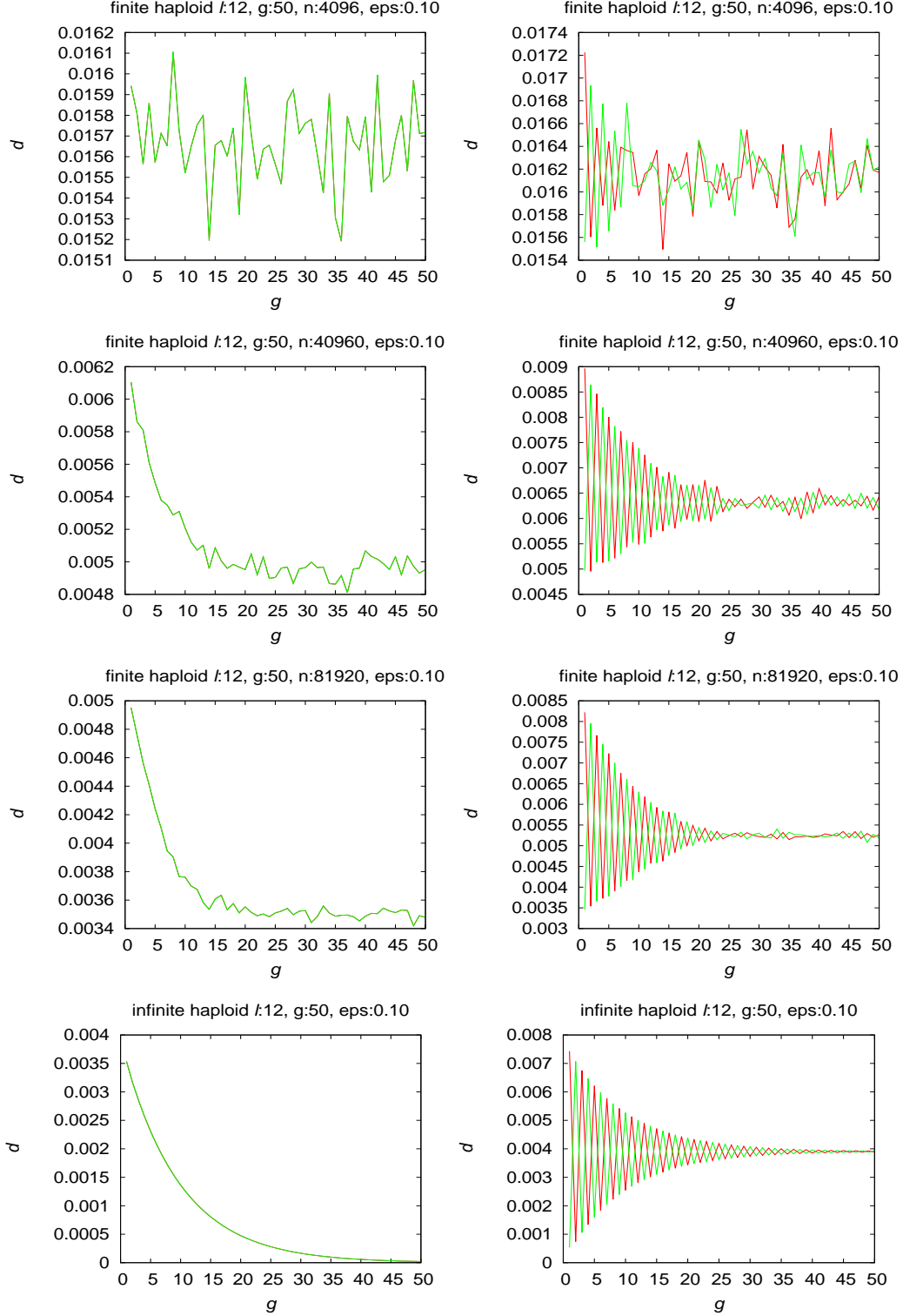
**Figure 3.45: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 10$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



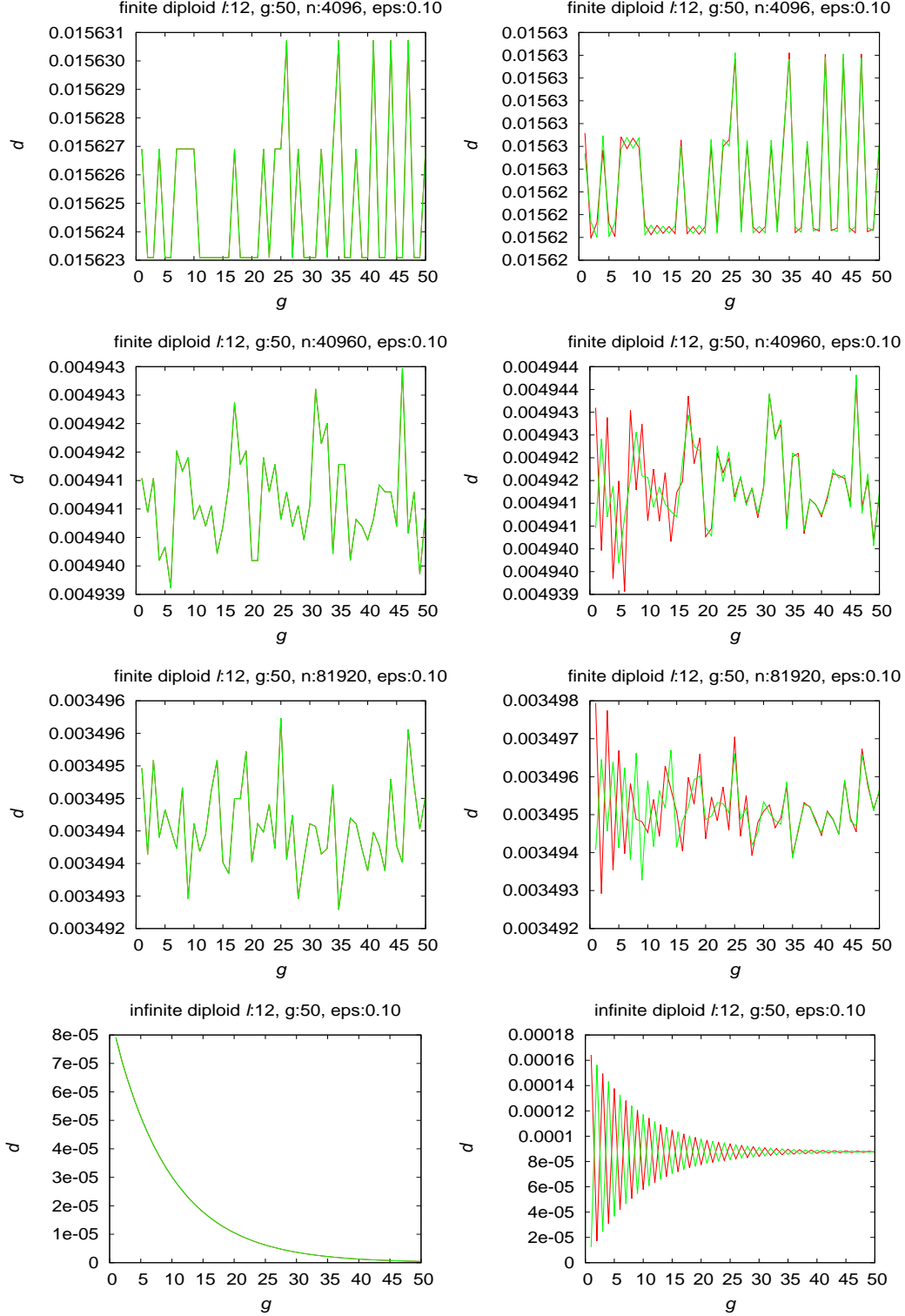
**Figure 3.46: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 12$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



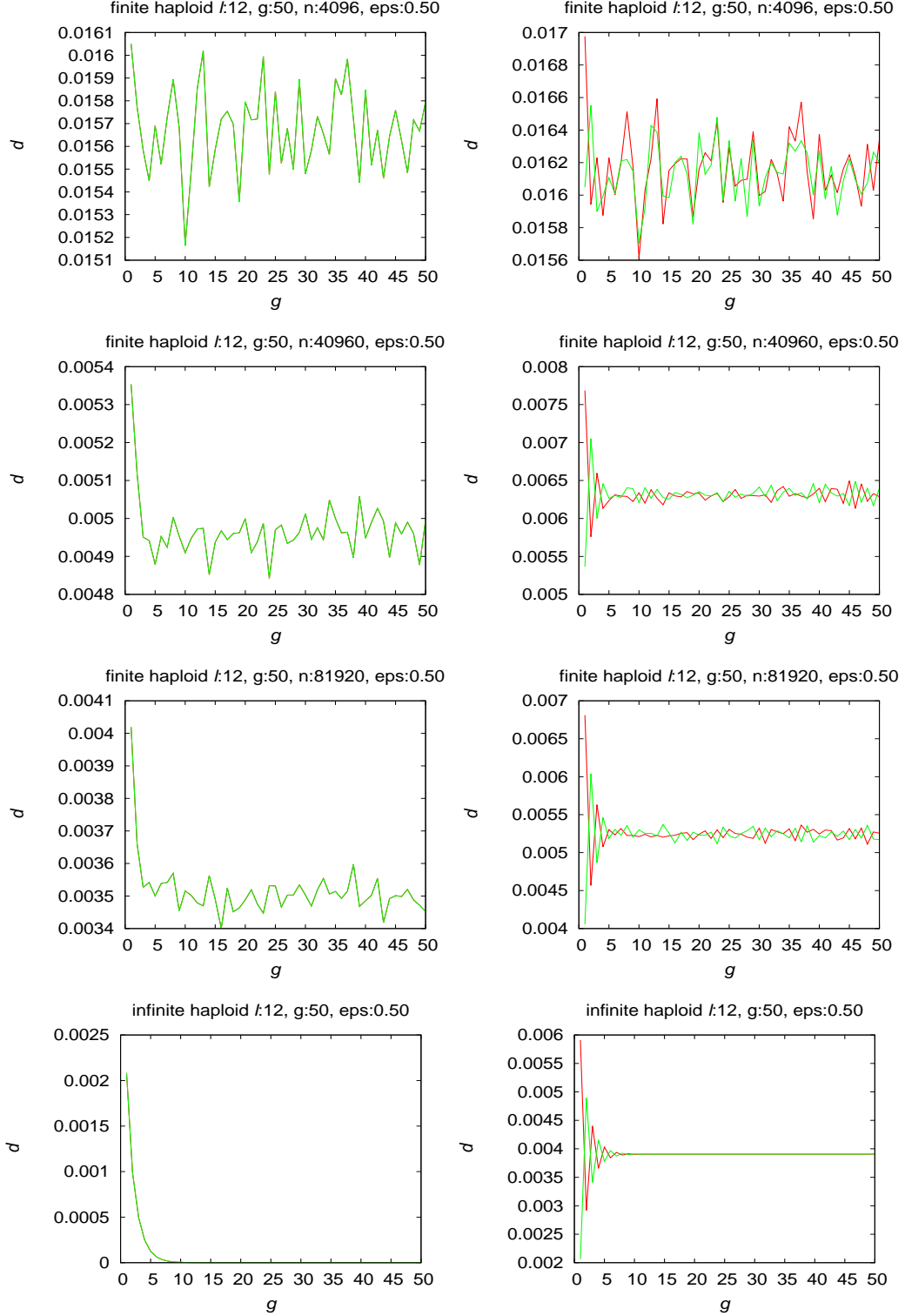
**Figure 3.47: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 12$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



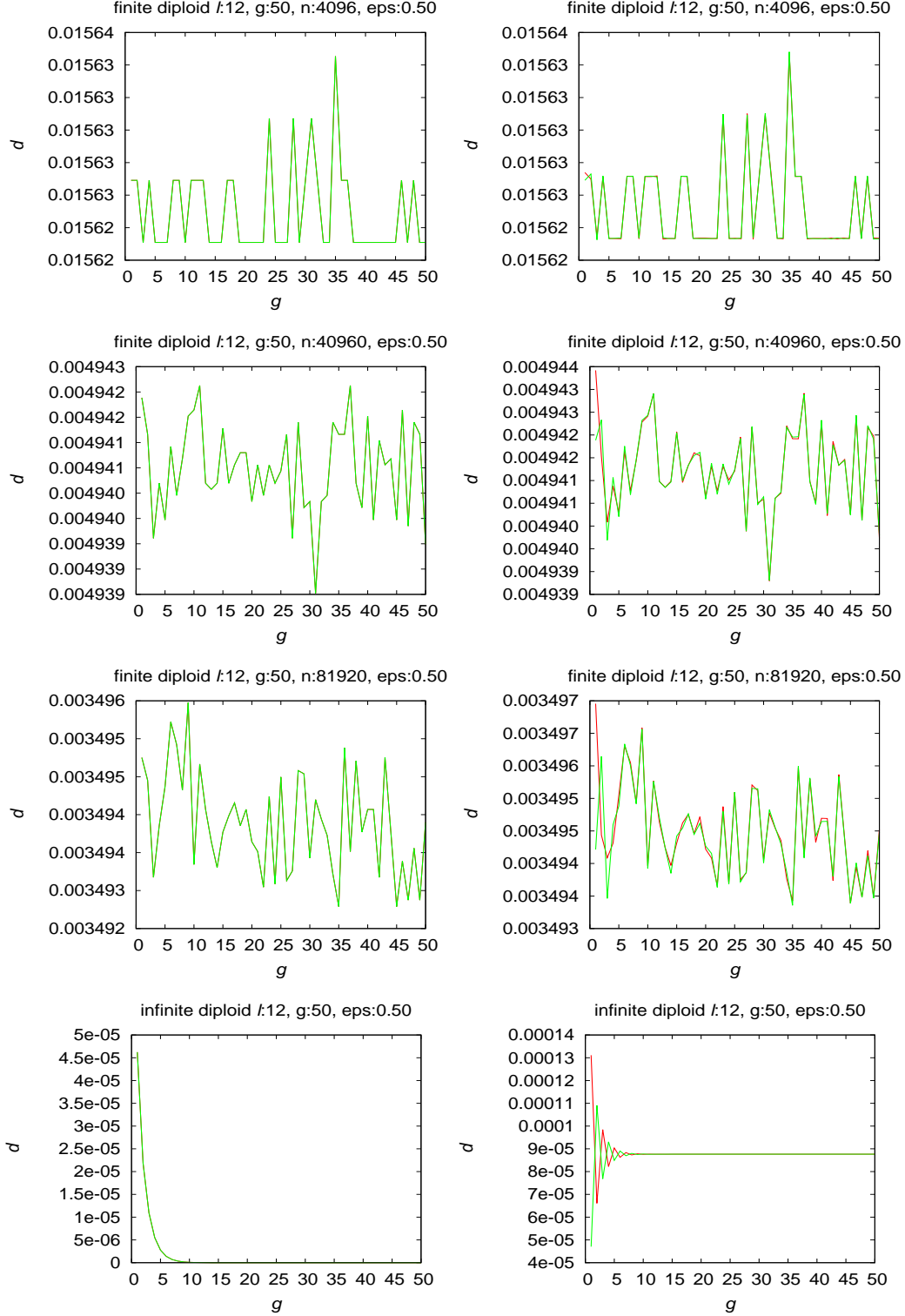
**Figure 3.48: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 12$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



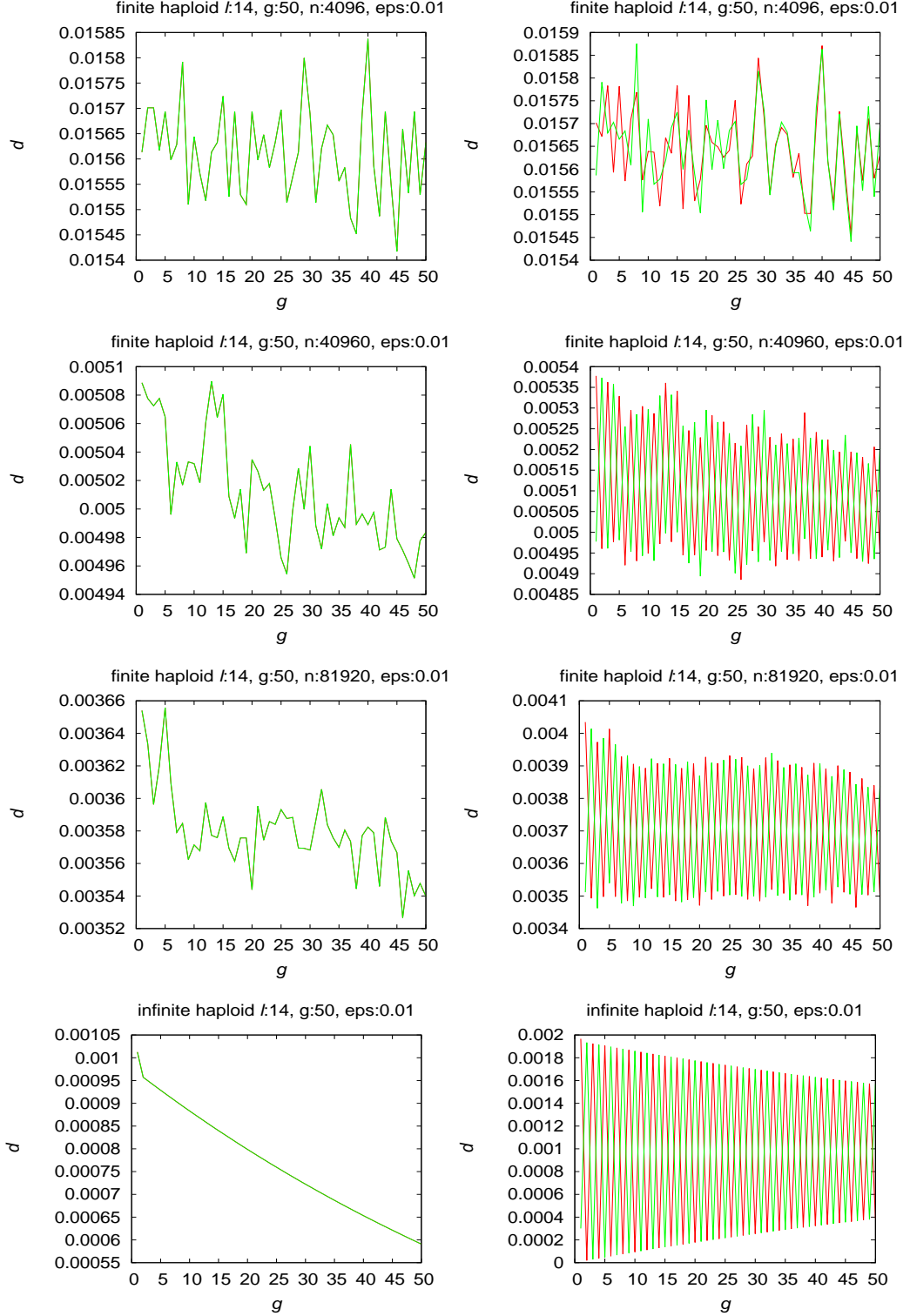
**Figure 3.49: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 12$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



**Figure 3.50: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 12$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

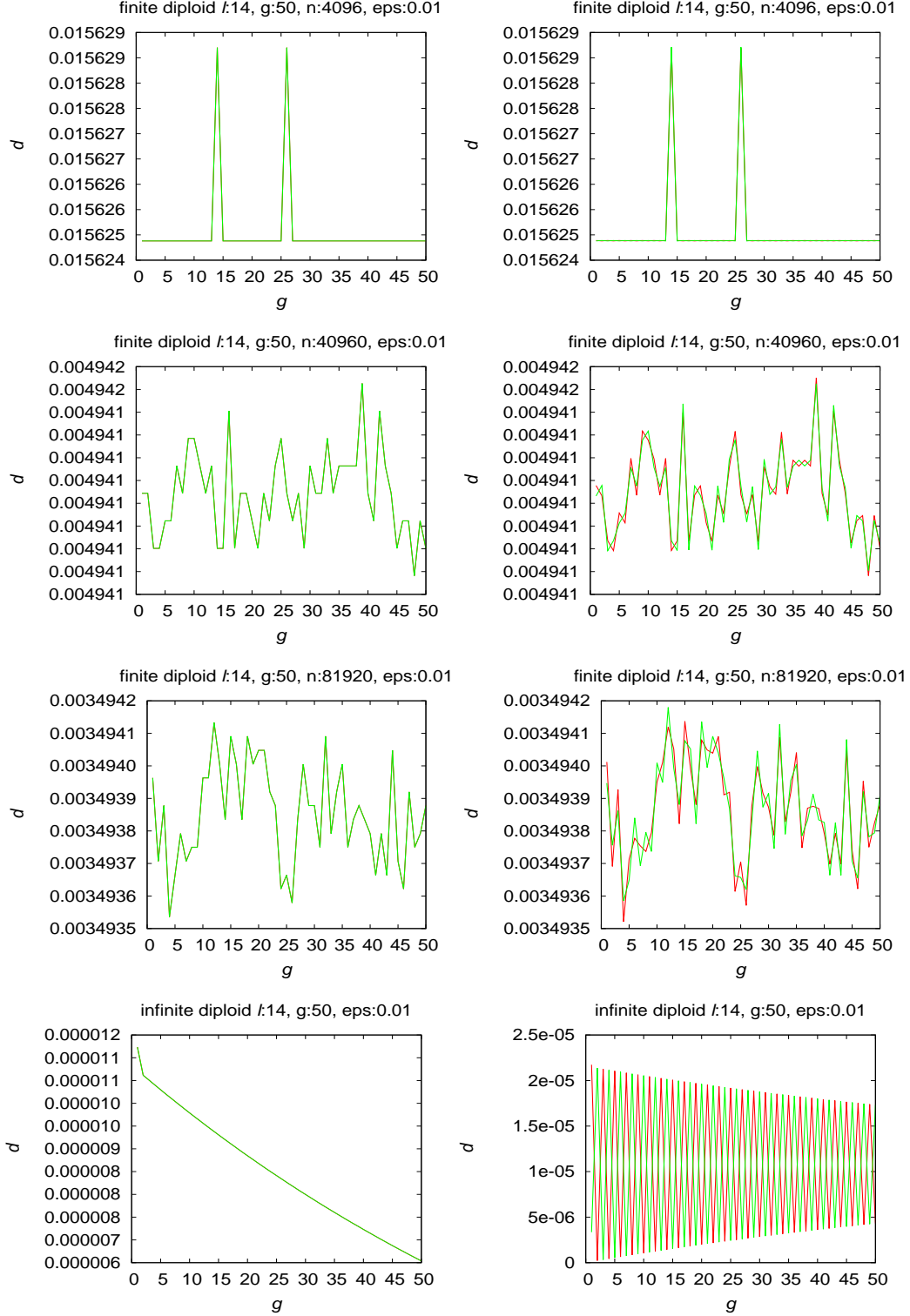


**Figure 3.51: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 12$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

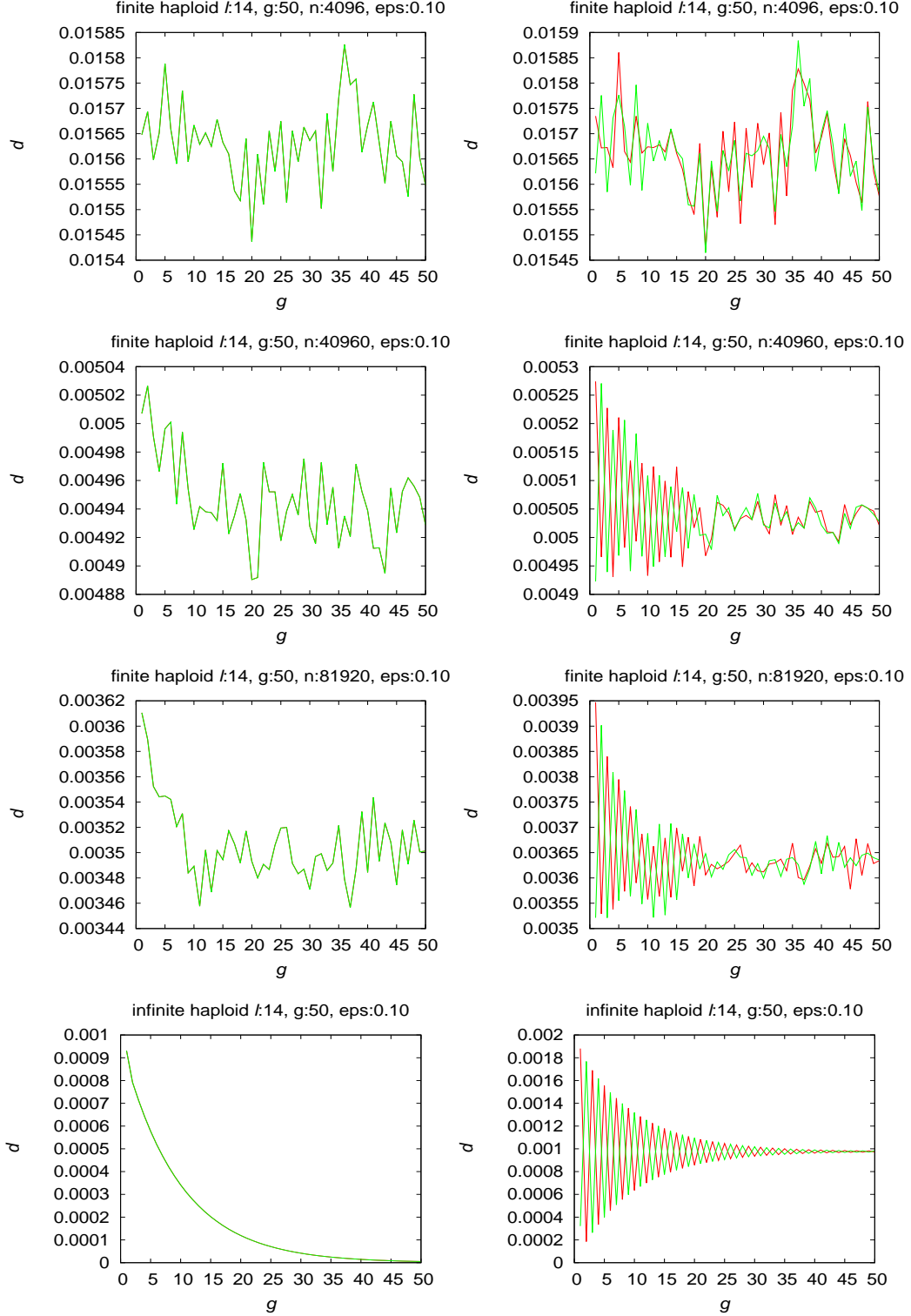


**Figure 3.52: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 14$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

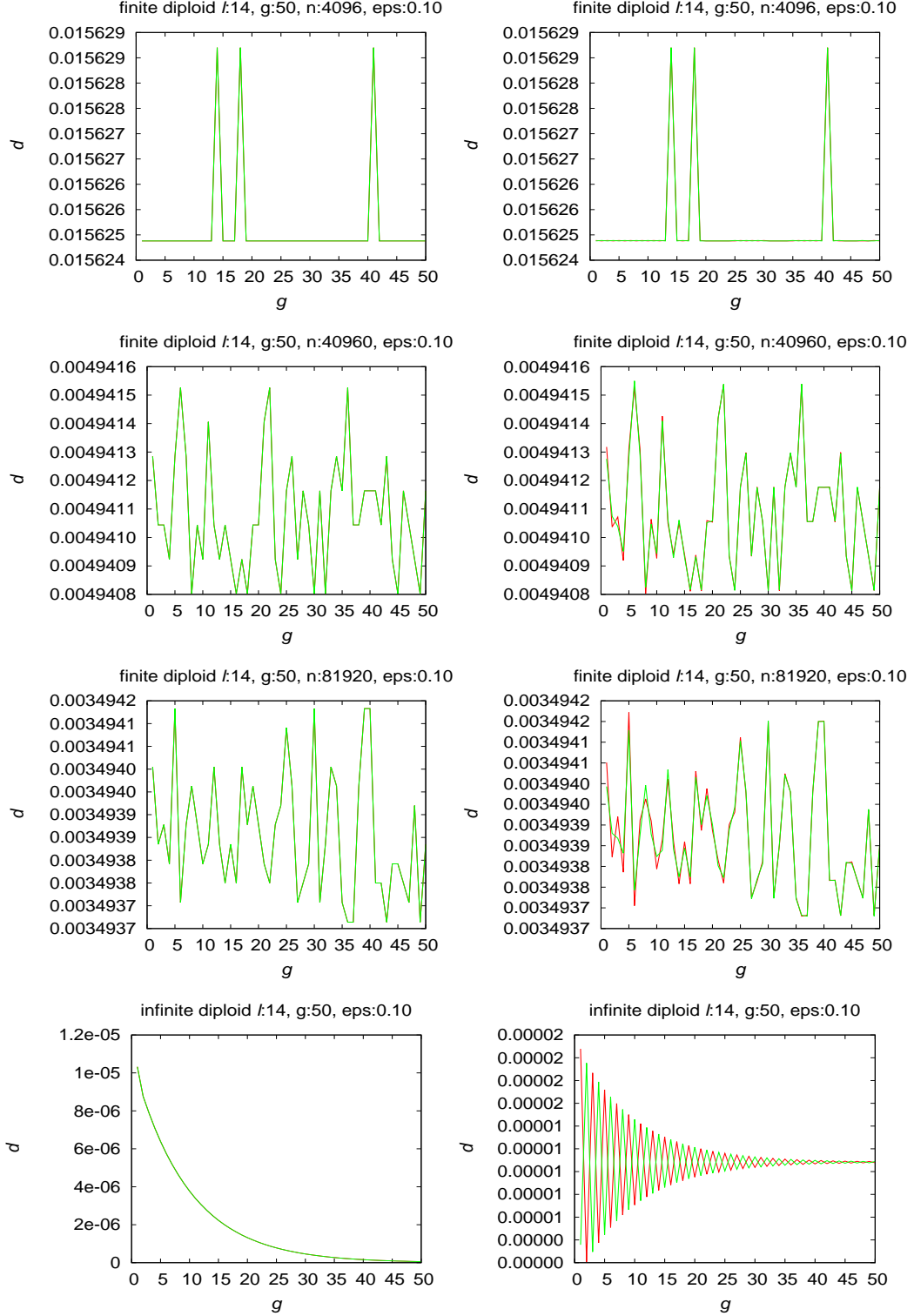




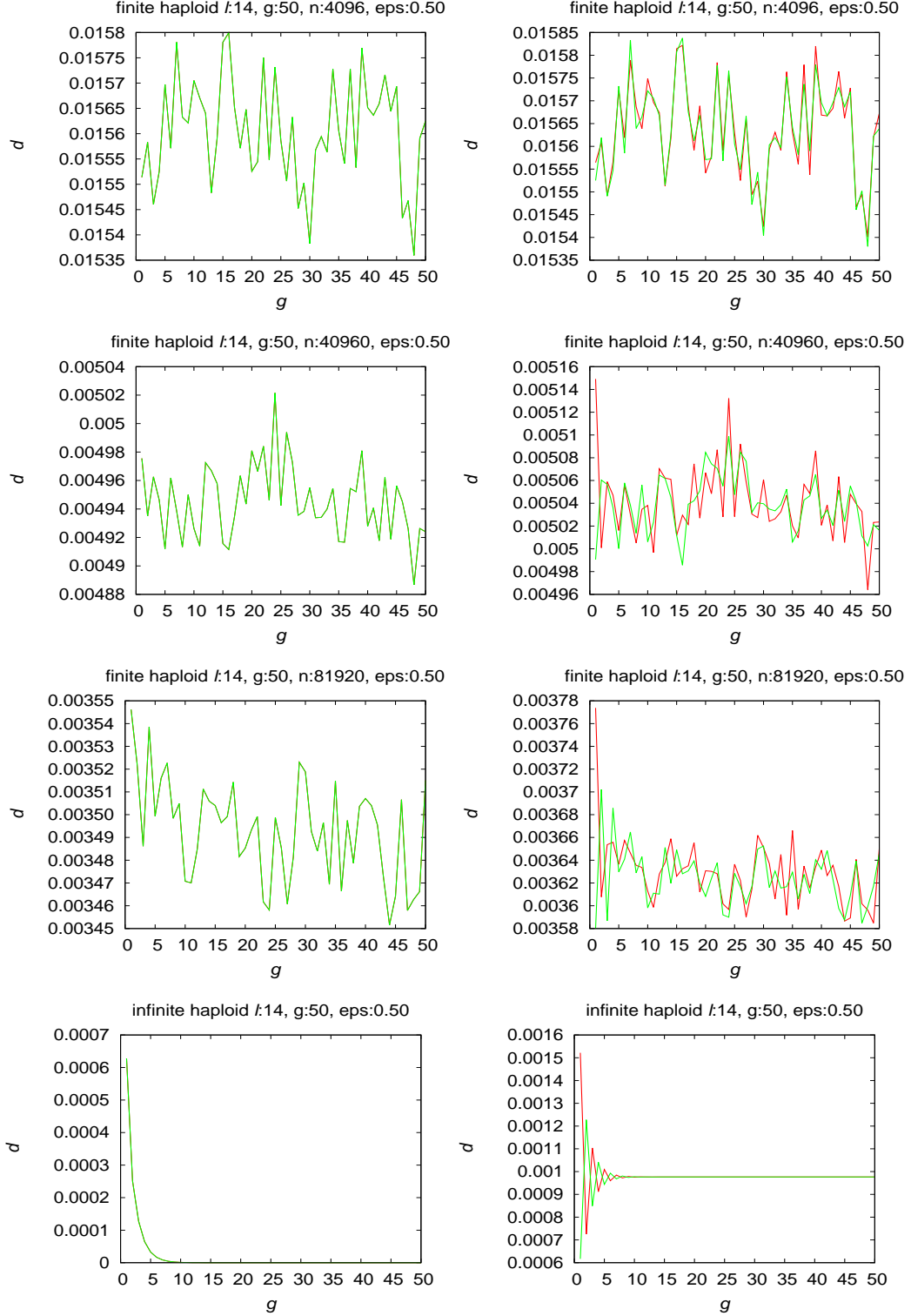
**Figure 3.53: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 14$  and  $\epsilon = 0.01$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



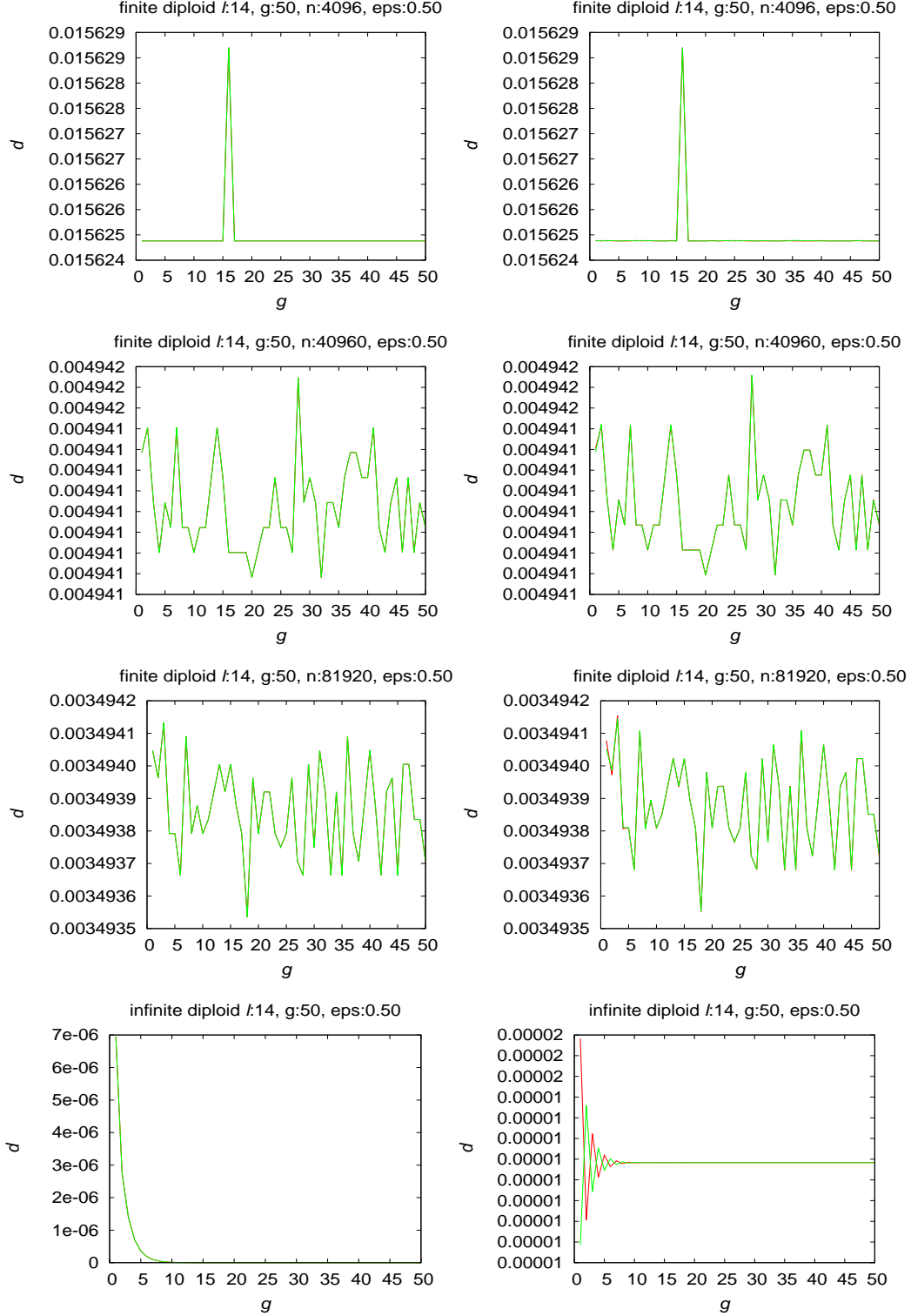
**Figure 3.54: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 14$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



**Figure 3.55: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 14$  and  $\epsilon = 0.1$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



**Figure 3.56: Infinite and finite haploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 14$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.



**Figure 3.57: Infinite and finite diploid population oscillation behavior in case of violation in  $\chi$  for genome length  $\ell = 14$  and  $\epsilon = 0.5$ :** In left column,  $d$  is distance of finite population of size  $n$  or infinite population to limit for  $g$  generations. In right column,  $d$  is distance of finite population of size  $N$  or infinite population to limits without violation.

Left column of graphs in above figures for violation in  $\mu$  and in  $\chi$  shows distance of finite and infinite population to evolutionary limits with violation and right column shows distance finite and infinite population to evolutionary limits without violation.

Graphs in right column give picture of oscillating behavior of population in presence of violation in  $\mu$  or  $\chi$  distribution where distance of population to limits with no violation. Both finite and infinite population oscillate in presence of violation, however, in case of infinite population, ripples die out quickly as generation increases and ceases to oscillate, giving graph a tapering shape and in case of finite population, even though amplitudes of ripples decreased, ripples didn't die out completely.

Change in oscillating behavior of population with change in  $\epsilon$  values  $\{0.01, 0.1, 0.5\}$  were also studied. Results show ripples damp out faster with increase  $\epsilon$ . With smaller values of  $\epsilon$ , oscillations were sharper and as value of  $\epsilon$  increased, rate of damping of ripples was quicker. Error  $\epsilon$  introduced to  $\mu$  or  $\chi$  distribution creates new masks (different than in case of without violation) to be used in mutation or crossover during transmission. With small  $\epsilon$ , the probability of using the new masks available due to violation is very small and those masks might not be used at all during crossover or mutation in finite population and with higher values of  $\epsilon$ , those new masks have higher chance of usage during mutation or crossover which cause oscillation to damp out quickly or cause no oscillation at all. In figures for violation in  $\mu$  distribution, with  $\epsilon = 0.01$ , oscillation is clearly visible and ripples are sharper; with  $\epsilon = 0.1$  oscillation was visible but ripples were damping out quickly; with  $\epsilon = 0.5$ , oscillation was very minimal or not visible at all. As population size increases, chance of new masks created due to violation in  $\mu$  or  $\chi$  distribution also increases, thus, ripples damp out more quickly.

Graphs in left column show distance between finite population and limit  $z^*$  with violation decreases as finite population size increases and shows behavior similar to infinite population behavior as finite population reach large number. Simulation results show infinite population converges to limit  $z^*$  quicker with increase in  $\epsilon$ . The

distance data in case of both  $\mu$  and  $\chi$  distribution violation with different values of  $\epsilon$  for different finite population size  $N$  are tabulated below.

**Table 3.3: Experimental distance measured for violation in  $\mu$ :**  $\ell$  is genome length,  $\epsilon$  is error introduced to  $\mu$  for violation,  $\{d', d'', d'''\}$  are distance measured for population size  $\{4096, 40960, 81920\}$  respectively

$\epsilon$	case	$\ell$	$d'$	$d''$	$d'''$
0.01	haploid	8	0.017614	0.009411	0.009261
		10	0.016812	0.008761	0.007667
		12	0.016099	0.006417	0.005315
		14	0.015690	0.005141	0.003821
	diploid	8	0.015635	0.004994	0.003582
		10	0.015631	0.004952	0.003508
		12	0.015625	0.004942	0.003495
		14	0.015625	0.004941	0.003494
0.1	haploid	8	0.015805	0.005400	0.004080
		10	0.015825	0.005281	0.003938
		12	0.015672	0.005064	0.003649
		14	0.015645	0.004969	0.003541
	diploid	8	0.015631	0.004946	0.003499
		10	0.015623	0.004942	0.003508
		12	0.015625	0.004941	0.003495
		14	0.015625	0.004941	0.003494
0.5	haploid	8	0.016364	0.005641	0.004239
		10	0.016130	0.005491	0.004048
		12	0.015743	0.005079	0.003642
		14	0.015736	0.005109	0.003684
	diploid	8	0.015630	0.004952	0.003513
		10	0.015626	0.004944	0.003497
		12	0.015626	0.004941	0.003494
		14	0.015625	0.004941	0.003494



**Table 3.4: Experimental distance measured for violation in  $\chi$ :**  $\ell$  is genome length,  $\epsilon$  is error introduced to  $\chi$  for violation,  $\{d', d'', d'''\}$  are distance measured for population size  $\{4096, 40960, 81920\}$  respectively

$\epsilon$	case	$\ell$	$d'$	$d''$	$d'''$
0.01	haploid	8	0.018631	0.015022	0.011465
		10	0.015839	0.006201	0.005093
		12	0.015834	0.005639	0.004518
		14	0.015614	0.005012	0.003579
	diploid	8	0.015655	0.005064	0.003658
		10	0.015625	0.004945	0.003498
		12	0.015625	0.004942	0.003494
		14	0.015625	0.004941	0.003494
0.1	haploid	8	0.016264	0.006084	0.005129
		10	0.015677	0.005131	0.003709
		12	0.015671	0.005087	0.003667
		14	0.015632	0.004946	0.003506
	diploid	8	0.015617	0.004958	0.003518
		10	0.015625	0.004941	0.003494
		12	0.015625	0.004941	0.003494
		14	0.015625	0.004941	0.003494
0.5	haploid	8	0.015636	0.005062	0.003629
		10	0.015528	0.004944	0.003529
		12	0.015673	0.004968	0.003515
		14	0.015604	0.004945	0.003493
	diploid	8	0.015631	0.004942	0.003500
		10	0.015626	0.004941	0.003494
		12	0.015625	0.004941	0.003494
		14	0.015625	0.004941	0.003494

From table 3.3, average distance calculated for finite population size 4096 is 0.015861, for size 40960 is 0.005464 and for size 81920 is 0.004123. From table 3.4, average distance calculated for finite population size 4096 is 0.015797, for size 40960 is 0.005520 and for size 81920 is 0.004040. These results show experimental distance between finite population and the limit with violation closely follows expected single step distance between finite and infinite population given by 3.1 and the distance decreased as  $1/\sqrt{N}$ .

# Chapter 4

## Conclusion

This research shows how Vose's haploid model for Genetic Algorithms extends to the diploid case, improving the computation of infinite population evolutionary trajectories by significantly reducing the time and space used. Efficiency is achieved through decoupling haploid evolution from the evolution of infinite diploid populations and employing Walsh transform methods to compute the effects of mask-based crossover and mutation. The efficient computation of distance between finite and infinite diploid populations is achieved by leveraging the reduction from diploid to haploid case.

Simulations are thereby made feasible which otherwise would require excessive resources, as illustrated through computations confirming the convergence of finite diploid population short-term behaviour to the behaviour predicted by the diploid model. Results agree with the expected rate of convergence for the single-step haploid case; distance is inversely proportional to square root of population size.

todo: write conclusion about evolutionary limits

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# Appendix

# Vita

Vita goes here...