ON THE CONVERGENCE AND APPLICATIONS OF GENERALIZED SIMULATED ANNEALING*

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Abstract. The convergence of the generalized simulated annealing with time-inhomogeneous communication cost functions is discussed. This study is based on the use of log-Sobolev inequalities and semigroup techniques in the spirit of a previous article by one of the authors. We also propose a natural test set approach to study the global minima of the virtual energy. The second part of the paper is devoted to the application of these results. We propose two general Markovian models of genetic algorithms and we give a simple proof of the convergence toward the global minima of the fitness function. Finally we introduce a stochastic algorithm that converges to the set of the global minima of a given mean cost optimization problem.

Key words. simulated annealing, genetic algorithms, stochastic optimization

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Introduction. Let E be a finite state space and q an irreducible Markov kernel. The main purpose of this paper is to study the limiting behavior of a large class of time-inhomogeneous Markov processes controlled by two parameters $(\gamma, \beta) \in \mathbb{R}^2_+$ and associated with a family of Markov kernels $Q_{\gamma,\beta}(x,y)$ having the following property:

(1)
$$\exists k > 0 : k^{-1} q(x,y)e^{-\beta V_{\gamma}(x,y)} \le Q_{\gamma,\beta}(x,y) \le k q(x,y)e^{-\beta V_{\gamma}(x,y)},$$

where $V: \mathbb{R}_+ \times E^2 \to \mathbb{R}_+ \cup \{\infty\}$, $V_{\gamma}(x,y) < +\infty \iff q(x,y) > 0$, and for any $x,y \in E$, $(\gamma,\beta) \to Q_{\gamma,\beta}(x,y) \in C^1$.

For a discussion on the origins of this problem the reader is referred to the introduction of Trouvé [12], who studies the asymptotic behavior of such chains, with time-homogeneous function V(x,y), using large deviation techniques. The fundamental notions here are those of the log-Sobolev constant $a(\gamma,\beta)$ of $Q_{\gamma,\beta}$ and the relative entropy of a measure with respect to another measure. Other complementary results relating to time-inhomogeneous communication cost function can be found in Frigerio-Grillo [7], Younes [13], and more recently in Löwe [9], where Sobolev inequalities rather than log-Sobolev inequalities are used for classical models where q is assumed to be reversible and V_{γ} is associated with an a priori potential depending on γ .

For a probability measure m on E, inverse-freezing schedule $\beta \in C^1(\mathbb{R}_+, \mathbb{R}_+)$ and $\gamma \in C^1(\mathbb{R}_+, \mathbb{R}_+)$, we denote (Ω, P, F_t, X_t) as the canonical process associated with the family of generators $(L_{\gamma_t,\beta_t})_{t\geq 0} = (Q_{\gamma_t,\beta_t} - I)_{t\geq 0}$ whose initial condition is $m_0 = m$, and we denote m_t as the distribution of X_t .

The aim of section 1.1 is to give several conditions on the rate of increase of $\gamma_t, \beta_t \to +\infty$ to ensure the entropy of m_t with respect to π_{γ_t, β_t} converges to 0. We shall examine as much of the theory as possible in a form applicable to general optimization problems and applicable in particular to mean cost optimization problems.

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To illustrate our results we will restrict attention to various special classes of generalized simulated annealing. We will commence with a detailed analysis of general Markov kernels of the form

(2)
$$Q_{\beta}(x,y) = \sum_{u \in U} \overline{q}_{\beta}(x,u,y)e^{-\beta \overline{V}(x,u,y)},$$

where U is a given finite set, $\overline{V}: E \times U \times E \to \mathbb{R}_+$, and $\overline{q}_{\beta}: E \times U \times E \to \mathbb{R}_+$, $\beta \in \mathbb{R}_+$, is a family of functions satisfying some continuity and irreducibility conditions. This situation can be formulated in the general form (1). We will settle this question and provide the explicit computation of the corresponding communication cost function V. In a final stage we will give several conditions on the rate of decrease of the cooling schedule to ensure the convergence in probability of the corresponding canonical process X_t , as $t \to +\infty$, to the set of global minima of the virtual energy associated with V.

Another application is the situation in which the Markov kernel $Q_{\gamma,\beta}$ has the form

$$Q_{\gamma,\beta}(x,y) = q_{\beta}(x,y) e^{\beta V_{\gamma}(x,y)}$$

with

$$\lim_{\gamma \to +\infty} V_{\gamma}(x, y) = V(x, y), \qquad \lim_{\beta \to +\infty} q_{\beta}(x, y) = q(x, y)$$

for some Markov kernel q and some function $V: E \times E \to \mathbb{R}^+$. In this situation, let π_{β} be the unique invariant probability measure of the Markov generator $L_{\beta} = Q_{\beta} - I$, where

$$Q_{\beta}(x,y) = q(x,y) e^{-\beta V(x,y)}.$$

We will give several conditions on the rate of decrease of the cooling schedule and on the rate of convergence $\lim_{t\to+\infty} V_{\gamma_t} = V$ to ensure the entropy of m_t with respect to π_{β_t} converges to 0.

The above results imply that the canonical process X_t converges in law to the set of the global minima V^* of a virtual energy V. This leads us to investigate more closely the properties of such function. Section 1.2 introduces a natural test set approach to study V^* . Specifically, we will give a condition for a given subset $H \subset E$ to contain V^* .

Section 2 is devoted to application of these results, an area of which is the situation in which Q_{β} is the transition probability kernel of a genetic algorithm. Such algorithms can be formulated by a Markov process with state space $E = S^N$ (N > 1 and S a finite set) and whose transition probabilities Q_{β} includes a mutation transition $Q_{\beta}^{(1)}$ and a selection mechanism $Q_{\beta}^{(2)}$. More precisely the mutation transition is modeled by independent motion of each particle and the selection mechanism chooses randomly in the previous population according to a given fitness function. The first convergence result was obtained by Cerf [2] in the case in which $Q_{\beta} = Q_{\beta}^{(1)} Q_{\beta}^{(2)}$ and the mutations vanish, that is, $\lim_{\beta \to +\infty} Q_{\beta}^{(1)}(x,y) = 1_x(y)$.

In section 2.1 we will use the results of section 1.1 and the test set approach introduced in section 1.2 to derive a new and simple proof of the convergence in probability of such algorithms to the set of the global minima of the fitness function in the following situations:

$$Q_{\beta} = Q_{\beta}^{(1)} Q_{\beta}^{(2)} \quad \text{and} \quad Q_{\beta} = \alpha \, Q_{\beta}^{(1)} + (1 - \alpha) \, Q_{\beta}^{(2)}, \quad 0 < \alpha < 1.$$

Finally, in subsection 2.2 we will apply the results of the first section to mean cost optimization problems. However, here we touch upon a slightly different aspect of the theory. Namely, the object will be to find the global minima of a function $U: E \to \mathbb{R}_+$ defined by

$$U(x) = E(L(Z, x)),$$

where Z is a random variable taking values in a finite set F and $L: F \times E \to \mathbb{R}_+$. We will solve this optimization problem by an original method based on the use of Monte Carlo simulations coupled with simulated annealing. This special case will require specific developments because the corresponding function V_{γ} will necessarily behave as a random process. We will present a time-inhomogeneous Markov process which converges to the global minima of U.

1. General results. The purpose of this section is to study the limiting behavior of time-inhomogeneous Markov chains controlled by two parameters $(\gamma, \beta) \in \mathbb{R}^2_+$ and associated with a family of Markov kernels $Q_{\gamma,\beta}(x,y)$ having the property (1), with the assumptions given in the introduction. This is in keeping with our second objective, which is to introduce some areas in which such results are useful.

The reader who is especially interested in genetic algorithms has to consult Corollary 1 and Propositions 3 and 4. Finally, the numerical solving of mean cost optimization problems requires only the use of Theorem 2 or Corollary 4.

1.1. Relative entropy convergence. Our analysis will be based entirely on considerations of the time-continuous semigroup associated with the Markov kernels $Q_{\gamma,\beta}(x,y)$ introduced in (1). Namely, define for $f: E \to \mathbb{R}$

$$L_{\gamma,\beta}f(x) = \sum_{y \in E} (f(y) - f(x)) Q_{\gamma,\beta}(x,y).$$

For a probability measure m on E, an inverse-freezing schedule $\beta \in C^1(\mathbb{R}_+, \mathbb{R}_+)$, and $\gamma \in C^1(\mathbb{R}_+, \mathbb{R}_+)$, we denote (Ω, P, F_t, X_t) as the canonical process associated with the family of generators $(L_{\gamma_t,\beta_t})_{t\geq 0} = (Q_{\gamma_t,\beta_t} - I)_{t\geq 0}$ whose initial condition is $m_0 = m$, and we write m_t the distribution of X_t .

Whenever X is time-homogeneous (i.e., $\beta_t = \beta$ and $\gamma_t = \gamma$) it is well known that $L_{\gamma,\beta}$ has a unique invariant probability measure $\pi_{\gamma,\beta}$ so that

$$\forall f: E \to \mathbb{R} \qquad \pi_{\gamma,\beta}(L_{\gamma,\beta}f) = 0$$

and $\pi_{\gamma,\beta}$ charges all the points. It is also convenient to recall the notion of log-Sobolev constant of $Q_{\gamma,\beta}$. Namely,

$$a(\gamma, \beta) \stackrel{\text{def}}{=} \min \left\{ \mathcal{E}_{\gamma, \beta}(f, f) / \mathcal{L}_{\gamma, \beta}(f), \ \mathcal{L}_{\gamma, \beta}(f) \neq 0 \right\},$$

where the Dirichlet form $\mathcal{E}_{\gamma,\beta}$ and $\mathcal{L}_{\gamma,\beta}$ are defined by

$$\mathcal{E}_{\gamma,\beta}(f,g) = -\langle L_{\gamma,\beta}f, g\rangle_{\pi_{\gamma,\beta}} = -\sum_{x \in E} L_{\gamma,\beta}f(x) \ g(x) \ \pi_{\gamma,\beta}(x),$$
$$\mathcal{L}_{\gamma,\beta}(f) = \sum_{x \in E} f(x)^2 \log\left(f(x)^2 / \|f\|_{2,\pi_{\gamma,\beta}}^2\right) \pi_{\gamma,\beta}(x).$$

Let us recall the notion of relative entropy of a measure m with respect to a measure π charging all the points

$$\operatorname{Ent}_{\pi}(m) = \sum_{x \in E} m(x) \, \log \left(m(x) / \pi(x) \right).$$

Using this notation, whenever X is time-homogeneous, one has the following basic inequality (for instance, see Miclo [10]):

(3)
$$\frac{d}{dt} \operatorname{Ent}_{\pi_{\gamma,\beta}}(m_t) \le -2 \ a(\gamma,\beta) \ \operatorname{Ent}_{\pi_{\gamma,\beta}}(m_t).$$

For an expository paper on log-Sobolev constants for the general Markov chain on finite spaces the reader is referred to Diaconis–Saloff-Costes [5]. Holley and Stroock [8] use Sobolev and log-Sobolev inequalities to study the standard simulated annealing. For another approach using only spectral gap estimates the reader should consult [4]. Using log-Sobolev inequalities, one of the authors addressed the convergence of a simulated annealing associated with a Markov transition kernel of the form using the entropy distance to stationarity (see [10]). The purpose of this section is to extend these results to general Markov transition kernels of form (1).

What follows is an exposition of some basic results regarding the description of $\pi_{\gamma,\beta}$, by Bott-Mayberry [1] and also exposed in Freidlin-Wentzell [6]. For $x \in E$ we denote $G_E(x)$, or G(x) when there are no possible confusions, as the set of x-graphs. We shall also use the following notations for $x \in E$ and $g \in G(x)$:

$$R_{\gamma,\beta}(x) = \sum_{g \in G(x)} Q_{\gamma,\beta}(g), \qquad Q_{\gamma,\beta}(g) = \prod_{(y \to z) \in g} Q_{\gamma,\beta}(y,z),$$
$$V_{\gamma}(g) = \sum_{(y \to z) \in g} V_{\gamma}(y,z), \qquad \mathbf{Q}_{\gamma,\beta}(x,y) = q(x,y) \ e^{-\beta \ V_{\gamma}(x,y)}.$$

Then, whenever X is time-homogeneous, its invariant distribution $\pi_{\gamma,\beta}$ is given by

$$\pi_{\gamma,\beta}(x) = R_{\gamma,\beta}(x) / \sum_{z \in E} R_{\gamma,\beta}(z).$$

Similarly, let $\mu_{\gamma,\beta}$ be the invariant probability measure of

$$\mathbf{L}_{\gamma,\beta}f(x) = \sum_{y \in E} (f(y) - f(x)) \ \mathbf{Q}_{\gamma,\beta}(x,y).$$

If $\mathbf{a}(\gamma, \beta)$ is the log-Sobolev constant of $\mathbf{Q}_{\gamma,\beta}$, then under assumption (1) there exists some constant $k_1 > 0$ such that

(4)
$$k_1^{-1}\mu_{\gamma,\beta}(x) \le \pi_{\gamma,\beta}(x) \le k_1\mu_{\gamma,\beta}(x).$$

Now, from the very definition of $\mu_{\gamma,\beta}$ and (4), we have the estimate

$$-\beta^{-1} \log \pi_{\gamma,\beta}(x) \xrightarrow[\beta \to +\infty]{} V_{\gamma}(x) - \min_{z \in E} V_{\gamma}(z) \quad \text{with} \quad V_{\gamma}(x) \stackrel{\text{def}}{=} \min_{g \in G(x)} V_{\gamma}(g).$$

As a direct consequence of Lemma 3.3, Diaconis–Saloff-Costes [5], and the inequalities (1) and (4) there exists some constant B > 0 such that

$$B^{-1} \mathbf{a}(\gamma, \beta) \le a(\gamma, \beta) \le B \mathbf{a}(\gamma, \beta).$$

Finally, by Theorem 3.23 of Holley–Stroock [8] and the inequalities stated in Miclo [10], we have the following proposition.

Proposition 1. There exists some constant A > 0 such that $a(\gamma, \beta) \ge A \frac{e^{-\beta c(\gamma)}}{1+\beta}$, where $c(\gamma)$ is the critical height associated with the communication cost V_{γ} given by

$$\begin{split} c(\gamma) &= \max_{x,y \in E} \left(\min_{p \in \mathcal{S}_{x,y}} e_{\gamma}(p) - V_{\gamma}(x) - V_{\gamma}(y) \right) + \min_{z \in E} V_{\gamma}(z), \\ e_{\gamma}(p) &= \max_{1 \leq i \leq n} \min \left(V_{\gamma}(p_{i-1}) + V_{\gamma}(p_{i-1}, p_i), V_{\gamma}(p_i) + V_{\gamma}(p_i, p_{i-1}) \right), \end{split}$$

where $S_{x,y}$ is the set of all the finite sequences from x to y and $e_{\gamma}(p)$ denotes elevation of a path. It can also be shown that

$$c(\gamma) = \max_{x,y \in E} \left(\min_{p \in C_{x,y}} \tilde{e}_{\gamma}(p) - V_{\gamma}(x) - V_{\gamma}(y) \right) + \min_{z \in E} V_{\gamma}(z),$$

where

$$\tilde{e}_{\gamma}(p) = \max_{1 \le i \le n} V_{\gamma}(p_{i-1}) + V_{\gamma}(p_{i-1}, p_i)$$

and $C_{x,y}$ is the set of all paths (admissible for q) from x to y. By choosing $t \to (\gamma_t, \beta_t)$ to go to infinity and using (3) we arrive at

$$(5) \quad \frac{d}{dt} \operatorname{Ent}_{\pi_{\gamma_t,\beta_t}}(m_t) \le -2 A \frac{e^{-\beta_t c(\gamma_t)}}{1+\beta_t} \operatorname{Ent}_{\pi_{\gamma_t,\beta_t}}(m_t) - \sum_{\sigma, \Gamma} m_t(x) \frac{d}{dt} \log \pi_{\gamma_t,\beta_t}(x).$$

Therefore it remains to estimate the derivatives $d\pi_{\gamma,\beta}/d\beta$ and $d\pi_{\gamma,\beta}/d\gamma$. For this purpose, write

$$\overline{Q}_{\gamma,\beta}(g) = Q_{\gamma,\beta}(g) / \sum_{h \in I_x} Q_{\gamma,\beta}(h), \qquad I_x = \left\{ g \in G(x) : \prod_{(y \to z) \in g} q(y,z) > 0 \right\}.$$

By a simple analysis it is easily checked that

$$\begin{split} &\frac{d}{d\beta}\log R_{\gamma,\beta}(x) = \sum_{g \in I_x} \overline{Q}_{\gamma,\beta}(g) \frac{d}{d\beta} \log Q_{\gamma,\beta}(g), \\ &\frac{d}{d\beta}\log \pi_{\gamma,\beta}(x) = \sum_{z \in F} \left(\frac{d}{d\beta} \log R_{\gamma,\beta}(x) - \frac{d}{d\beta} \log R_{\gamma,\beta}(z) \right) \pi_{\gamma,\beta}(z). \end{split}$$

In order to derive a useful inequality we assume there exist two functions $d_1, d_2 : \mathbb{R}_+ \to \mathbb{R}_+$ such that

(6)
$$\sup_{g \in \cup_x I_x} \frac{d}{d\beta} \log Q_{\gamma,\beta}(g) - \inf_{g \in \cup_x I_x} \frac{d}{d\beta} \log Q_{\gamma,\beta}(g) \le d_1(\gamma),$$

(7)
$$\sup_{g \in \cup_x I_x} \frac{d}{d\gamma} \log Q_{\gamma,\beta}(g) - \inf_{g \in \cup_x I_x} \frac{d}{d\gamma} \log Q_{\gamma,\beta}(g) \le d_2(\beta).$$

Note that by the very definitions of the sets I_x it clearly suffices to have

$$\left| \frac{d}{d\beta} \log Q_{\gamma,\beta}(x,y) \right| \le \tilde{d}_1(\gamma), \qquad \left| \frac{d}{d\gamma} \log Q_{\gamma,\beta}(x,y) \right| \le \tilde{d}_2(\beta)$$

for every q(x,y) > 0 and two functions \tilde{d}_1 , $\tilde{d}_2 : \mathbb{R}_+ \to \mathbb{R}_+$. Now we are ready to apply the following technical lemma.

LEMMA 1 (Stroock [11]). If μ is a probability measure and $\theta \in L^1(\mu)^+$ satisfies $\int \theta d\mu = 1$, then for every $\phi \in L^{\infty}(\mu)$ satisfying $\int \phi d\mu = 0$ one has

$$\left| \int \phi \, \theta \, d\mu \right| \leq \sqrt{2} \, \|\phi\|_{L^{\infty}(\mu)} \, \left(\int \, \theta \, \log \theta \, d\mu \right)^{1/2}.$$

Using this lemma with $\mu = \pi_{\gamma,\beta}$, $\phi = d \log \pi_{\gamma,\beta}/d\beta$ (resp., $\phi = d \log \pi_{\gamma,\beta}/d\gamma$), and $\theta = m_t/\pi_{\gamma_t,\beta_t}$ and writing

$$I_t \stackrel{\text{def}}{=} (\text{Ent}_{\pi_{\gamma_t,\beta_t}}(m_t))^{1/2}$$

we see from (5) that

(8)
$$\frac{dI_t}{dt} \le -A_0 \frac{e^{-\beta_t c(\gamma_t)}}{1+\beta_t} I_t + A_1 d_1(\gamma_t) \left| \frac{d\beta_t}{dt} \right| + A_2 d_2(\beta_t) \left| \frac{d\gamma_t}{dt} \right|$$

for some constants $A_0, A_1, A_2 > 0$. Hence by taking, for t sufficiently large, an inverse-temperature schedule of the form $\beta_t = K^{-1} \log t$ we obtain

$$\frac{dI_t}{dt} \le -A_t \ I_t + B_t$$

with

$$A_t = A_0 \ t^{-c(\gamma_t)/K} (1 + K^{-1} \log t)^{-1}$$
 and $B_t = A_1 \frac{d_1(\gamma_t)}{Kt} + A_2 d_2(K^{-1} \log t) \left| \frac{d\gamma_t}{dt} \right|$.

Now, it is well known that

$$\exists t_0 \in \mathbb{R}_+ \quad \int_{t_0}^{+\infty} A_s \ ds = +\infty, \qquad \lim_{t \to +\infty} \frac{B_t}{A_t} = 0 \Longrightarrow \lim_{t \to +\infty} I_t = 0.$$

We can now summarize the entire consideration in the following way.

THEOREM 1. Assume that $c = \limsup_{\gamma \to +\infty} c(\gamma) < +\infty$ and the conditions

$$\sup_{x \in E} \left| \frac{d}{d\beta} \mu_{\gamma,\beta}(x) \right| \le d_1(\gamma), \qquad \sup_{x \in E} \left| \frac{d}{d\gamma} \mu_{\gamma,\beta}(x) \right| \le d_2(\beta)$$

are satisfied for two nonnegative functions d_1 , d_2 .

When the inverse-freezing schedule has parametric form $\beta_t = K^{-1} \log t$, for t sufficiently large and K > c, we have

(9)
$$\lim_{t \to +\infty} \operatorname{Ent}_{\pi_{\gamma_t,\beta_t}}(m_t) = 0$$

whenever

(10)
$$\frac{d\gamma_t}{dt} = o\left(1/(d_2(\log t^{1/K})t^{c/K}\log t)\right), \qquad d_1(\gamma_t)/t = o\left(1/(t^{c/K}\log t)\right).$$

Remark. The hypothesis above might seem difficult to check; we shall see in fact that in many cases it is indeed fulfilled. In practice the Markov kernels $Q_{\gamma,\beta}$ are known and it clearly suffices to check that

$$\begin{split} \sup_{g \in \cup_x I_x} \frac{d}{d\beta} \log Q_{\gamma,\beta}(g) - \inf_{g \in \cup_x I_x} \frac{d}{d\beta} \log Q_{\gamma,\beta}(g) &\leq d_1(\gamma), \\ \sup_{g \in \cup_x I_x} \frac{d}{d\gamma} \log Q_{\gamma,\beta}(g) - \inf_{g \in \cup_x I_x} \frac{d}{d\gamma} \log Q_{\gamma,\beta}(g) &\leq d_2(\beta). \end{split}$$

Because of the general orientation provided in this section we can proceed immediately to review the most important special class of generalized simulated annealing, which we shall study later. Let us consider the transition probability kernels

(11)
$$Q_{\beta}(x,y) = \sum_{u \in U} \overline{q}_{\beta}(x,u,y)e^{-\beta \overline{V}(x,u,y)},$$

where U is a given finite set, $\overline{V}: U \times E^2 \to \mathbb{R}_+$, and $\overline{q}_{\beta}(x, u, y) \geq 0$. The proof of Theorem 1 shows it is important that the Markov kernel q is irreducible. For this purpose we will assume the existence of nonnegative functions $\overline{q}(x, u, y)$ so that

$$(\mathcal{C}) \qquad \overline{q}_{\beta}(x, u, y) > 0 \Longleftrightarrow \overline{q}(x, u, y) > 0, \qquad \lim_{\beta \to +\infty} \overline{q}_{\beta}(x, u, y) = \overline{q}(x, u, y),$$

and we will work with the following irreducibility condition:

$$(\mathcal{I}) \, \forall x, y \in E \quad \exists (p_k, u_k)_{1 \le k \le r} : \quad p_0 = x, \quad p_k \in E \, u_k \in U \, p_r = y \, \overline{q}(p_k, u_k, p_{k+1}) > 0.$$

Our immediate goal is to prove the following consequence of Theorem 1 which gives conditions assuring the convergence stated in Theorem 1 for a time-inhomogeneous Markov chain with transitions (11). This corollary is applied in section 2 to the convergence of genetic algorithms

COROLLARY 1. Assume \overline{q}_{β} and \overline{q} satisfy the continuity and irreducibility conditions (\mathcal{C}) and (\mathcal{I}) . Then, the transition probabilities

(12)
$$Q_{\beta}(x,y) = \sum_{u \in U} \overline{q}_{\beta}(x,u,y)e^{-\beta \overline{V}(x,u,y)}$$

satisfy the inequalities (1) with

$$\begin{split} V(x,y) &= \min_{u \in U(x,y)} \overline{V}(x,u,y), \qquad U(x,y) = \{u \in U \ : \ \overline{q}(x,u,y) > 0\}, \\ q(x,y) &= \sum_{u \in U^\star(x,y)} \overline{q}(x,u,y), \qquad U^\star(x,y) = \{u \in U(x,y) \ : \ \overline{V}(x,u,y) = V(x,y)\}. \end{split}$$

Let V be the virtual energy function corresponding to the above communication cost function

$$V(x) = \min_{g \in G(x)} \sum_{(y \to z)} V(y, z)$$

and let c be the corresponding critical height. In addition, suppose that for every $\overline{q}(x,u,y) > 0$ and for some $\beta_0 \geq 0$

(13)
$$\sup_{\beta \ge \beta_0} \left| \frac{d \log \overline{q}_{\beta}}{d\beta}(x, u, y) \right| < +\infty.$$

In this case, if m is a probability measure on E and if β_t assumes the parametric form $\beta_t = K^{-1} \log t$, for sufficiently large t, with K > c, then

$$\lim_{t \to +\infty} Ent_{\pi_{\beta_t}}(m_t) = 0 \qquad and \qquad \lim_{t \to +\infty} P(X_t \in V^*) = 1,$$

where (Ω, P, F_t, X_t) is the canonical process associated with the family of generators $(L_{\beta_t})_{t\geq 0} = (Q_{\beta_t} - I)_{t\geq 0}$ whose initial condition is $m_0 = m$, m_t is the distribution of X_t , π_{β} is the unique invariant probability measure of L_{β} , and

$$V^* = \{x \in E : V(x) = \min_E V\}.$$

Proof. Using the form of \overline{q}_{β} we have for some suitable function $\epsilon(\beta) \to 0$, as $\beta \to +\infty$,

$$(14) (1 - \epsilon(\beta)) K_{\beta}(x, y) \le Q_{\beta}(x, y) \le (1 + \epsilon(\beta)) K_{\beta}(x, y),$$

where

$$K_{\beta}(x,y) = \sum_{u \in U(x,y)} \overline{q}(x,u,y)e^{-\beta \overline{V}(x,u,y)}.$$

But now we have that

$$\begin{split} K_{\beta}(x,y) &= \sum_{u \in U^{\star}(x,y)} \overline{q}(x,u,y) \; e^{-\beta V(x,y)} \\ &+ e^{-\beta V(x,y)} \sum_{u \in U(x,y)-U^{\star}(x,y)} \overline{q}(x,u,y) \; e^{-\beta(\overline{V}(x,u,y)-V(x,y))} \\ &= q(x,y) e^{-\beta V(x,y)} + e^{-\beta V(x,y)} \sum_{u \in U(x,y)-U^{\star}(x,y)} \overline{q}(x,u,y) \; e^{-\beta(\overline{V}(x,u,y)-V(x,y))}. \end{split}$$

Thus, condition (\mathcal{I}) implies that q is irreducible. Furthermore, if we write

$$I = \{(x, y) \in E^2 : U(x, y) \neq \emptyset\},\$$

 $J = \{(x, u, y) \in E \times U \times E : (x, y) \in I \ u \in U(x, y)\}$

and

$$h_1 = \min_{(x,y)\in I} \sum_{u\in U(x,y)-U^{\star}(x,y)} \overline{q}(x,u,y)/q(x,y),$$

$$h_2 = \min_{(x,u,y): u\notin U^{\star}(x,y)} \overline{V}(x,u,y) - V(x,y),$$

then using (14) we get the system of inequalities

$$(1 - \epsilon(\beta)) \ q(x, y) \ e^{\beta V(x, y)} \le Q_{\beta}(x, y) \le (1 + \epsilon(\beta)) \ (1 + h_1 \ e^{-\beta h_2}) q(x, y) \ e^{\beta V(x, y)}.$$

To end the proof it remains to check condition (6). Choose q(x,y) > 0; after some computations we find

$$\left| \frac{d \log Q_{\beta}(x,y)}{d\beta} \right| \le \sup_{u \in U(x,y)} \left| \frac{d \log \overline{q}_{\beta}}{d\beta}(x,u,y) \right| + \sup_{u \in U(x,y)} \overline{V}(x,u,y).$$

Thus (13) implies (6), and using Theorem 1 the proof of the first assertion is complete. Examination of the invariant distribution of L_{β} soon yields that $\forall x \notin V^{\star}$ we have $\lim_{\beta \to +\infty} \pi_{\beta}(x) = 0$. Then, to prove the last assertion it is enough to recall the basic inequality

$$||m_t - \pi_{\beta_t}||_{TV}^2 \le 2 \operatorname{Ent}_{\pi_{\beta_t}}(m_t),$$

where $\|.\|_{TV}$ is the distance in total variation given by

$$\|\mu - \nu\|_{TV} = 2 \sup_{A \subset E} |\mu(A) - \nu(A)|.$$

It is quite clear from definition (12) that the following situations are covered:

$$Q_{\beta} = Q_{\beta}^{(1)} Q_{\beta}^{(2)}$$
 and $Q_{\beta} = \alpha Q_{\beta}^{(1)} + (1 - \alpha) Q_{\beta}^{(2)}$, $0 < \alpha < 1$.

In section 2 we will develop properties of both class of chains which we shall find includes, as a special case, the evolutionary processes studied by Cerf in [2]. For the sake of unity and to highlight issues specific to evolutionary processes, we give some examples to suggest how these results translate in this special situation.

Examples.

- 1. If $d_1(\gamma) = \gamma^p$ and $d_2(\beta) = \beta^q$ for some $p \ge 0$ and q > 0, it clearly suffices to choose $\gamma_t = \log t$.
- 2. Let us study a way to combine the transitions $Q_{\beta}^{(1)}, \dots, Q_{\beta}^{(r)}$ given by

$$Q_{\beta}^{(k)}(x,y) = q_{\beta}^{(k)}(x,y) \ e^{-\beta V^{(k)}(x,y)}, \qquad V^{(k)} : E^2 \to \mathbb{R}_+, \qquad q_{\beta}^{(k)}(x,y) \ge 0.$$

It is clear from (11) that the following situation is covered:

(a)
$$Q_{\beta}(x,y) = Q_{\beta}^{(1)} \dots Q_{\beta}^{(r)}(x,y) = \sum_{z_1,\dots,z_{r-1} \in E} Q_{\beta}^{(1)}(x,z_1) \dots Q_{\beta}^{(r)}(z_{r-1},y).$$

This situation can be formulated in the form (11) with $U = E^{r-1}$ and

$$\overline{q}_{\beta}(x, u, y) = q_{\beta}^{(1)}(x, u_1) \dots q_{\beta}^{(r)}(u_{r-1}, y),$$

$$\overline{V}(x, u, y) = V^{(1)}(x, u_1) + \dots + V^{(r)}(u_{r-1}, y).$$

Also from (11), the following situation is covered:

(b)
$$\tilde{Q}_{\beta}(x,y) = \sum_{k=1}^{r} \alpha_k \ Q_{\beta}^{(k)}(x,y)$$
 with $\sum_{k=1}^{r} \alpha_k = 1$.
This situation can be formulated in the form (11) with $E = \{1, \dots, r\}$ and

$$\overline{q}_{\beta}(x,u,y) = \alpha_u \, q_{\beta}^{(u)}(x,y), \qquad \overline{V}(x,u,y) = V^{(u)}(x,y).$$

Probabilistically and in precise language 1(a) has the interpretation of being the transition of a chain obtained through overlapping r-1 other chains, and 1(b) has the interpretation of being the transition of a chain obtained through choosing randomly at each step among r chains. Let us remark, by way of illustration, that it is also possible to consider a way of combining 1(a) and 1(b) that subsumes such parallel and series combinations. For instance, each transition probability $Q_{\beta}^{(k)}$ in the expression (a) may be of type (b) and conversely. As a result one has a great freedom in the design and the physical construction of the transition probabilities $Q_{\gamma,\beta}$, and they appear ideally suited to describe a large class of processes encountered in applications.

3. Let us examine the above example when r=2. In this situation we introduce the irreducibility condition $(\mathcal{I})'$

(15)
$$q^{(1)}$$
 irreducible and $\forall x \in E$ $q^{(2)}(x,x) > 0$

and the continuity condition (C)'

$$\lim_{\beta \to +\infty} q_{\beta}^{(k)}(x,y) = q^{(k)}(x,y), \quad q_{\beta}^{(k)}(x,y) = 0 \iff q^{(k)}(x,y) = 0 \quad \forall k = 1, 2,$$
(16)

where $q^{(k)}(x,y)$ are transition probability kernels such that

$$q^{(k)}(x,y) = 0 \Longleftrightarrow V^{(k)}(x,y) = +\infty \qquad \forall k = 1, 2.$$

In this situation the conditions (\mathcal{C}) and (\mathcal{I}) of Corollary 1 are satisfied. In addition, if we assume that for every k=1,2 and $q^{(k)}(x,y)$

$$\left| \frac{d \log q_{\beta}^{(2)}}{d\beta}(x, y) \right| < +\infty,$$

then the last condition (13) introduced in Corollary 1 is satisfied. COROLLARY 2. Suppose the Markov kernel of the chain has the form

$$Q_{\gamma,\beta} = q_{\beta}(x,y)e^{-\beta V_{\gamma}(x,y)}$$

with

$$q_{\beta}(x,y) = 0 \iff q(x,y) = 0, \qquad \lim_{\beta \to +\infty} q_{\beta}(x,y) = q(x,y)$$

and assume the following conditions are satisfied for every $\beta, \gamma \in \mathbb{R}_+$ and some constant d > 0:

$$c = \sup_{\gamma} c(\gamma) < +\infty, \qquad \sup_{g \in \cup_x I_x} V_{\gamma}(g) - \inf_{g \in \cup_x I_x} V_{\gamma}(g) \le d,$$

$$\sup_{g \in \cup_x I_x} \frac{d}{d\beta} \log q_{\beta}(g) - \inf_{g \in \cup_x I_x} \frac{d}{d\beta} \log q_{\beta}(g) \le d \sup_{g \in \cup_x I_x} \frac{d}{d\gamma} V_{\gamma}(g) - \inf_{g \in \cup_x I_x} \frac{d}{d\gamma} V_{\gamma}(g) \le d.$$

When the inverse freezing schedule has parametric form $\beta_t = K^{-1} \log t$, for t sufficiently large and K > c, we have

$$\lim_{t \to +\infty} \operatorname{Ent}_{\pi_{\gamma_t,\beta_t}}(m_t) = 0 \qquad \text{whenever} \quad \frac{d\gamma_t}{dt} = o(1/(t^{c/K} \log^2 t)).$$

As a consequence we have the well-known corollary that follows. COROLLARY 3 (Miclo [10]). Suppose the Markov kernel of the chain has the form

$$Q_{\gamma,\beta} = q(x,y)e^{-\beta V(x,y)} \stackrel{\text{def}}{=} Q_{\beta}(x,y).$$

When the inverse freezing schedule has parametric form $\beta_t = K^{-1} \log t$, for t sufficiently large and K > c, we have

$$\lim_{t \to +\infty} \operatorname{Ent}_{\pi_{\beta_t}}(m_t) = 0,$$

where π_{β} is the unique invariant probability measure of the Markov generator $Q_{\beta}-I$.

The usefulness of Theorem 1 will now be illustrated in the case where the transition probabilities $Q_{\gamma,\beta}$ converge to a transition probability kernel Q_{β} as $\gamma \to +\infty$.

THEOREM 2. Let $Q_{\beta}(x,y)$ be a Markov kernel such that $Q_{\beta}(x,y) = 0 \iff q(x,y) = 0$. Suppose the assumptions of Theorem 1 are satisfied and for every q(x,y) > 0

(17)
$$\lim_{t \to +\infty} |\log Q_{\gamma_t, \beta_t}(x, y) - \log Q_{\beta_t}(x, y)| = 0.$$

Then

(18)
$$\lim_{t \to +\infty} \operatorname{Ent}_{\pi_{\beta_t}}(m_t) = 0,$$

where π_{β} is the unique invariant probability measure of the Markov generator $Q_{\beta}-I$. Proof. By the same line of argument as before π_{β} may be described as follows:

$$\pi_{\beta}(x) = \frac{R_{\beta}(x)}{\sum_{z \in E} R_{\beta}(z)} \quad \text{with} \quad R_{\beta}(x) = \sum_{g \in I_x} Q_{\beta}(g) \quad \text{and} \quad Q_{\beta}(g) = \prod_{(y \to z) \in g} Q_{\beta}(y, z).$$

(19)

It follows that

$$\log \frac{\pi_{\gamma,\beta}}{\pi_{\beta}}(x) = -\log \left(\sum_{g \in I_x} \prod_{(y \to z) \in g} (Q_{\beta} Q_{\gamma,\beta}^{-1})(y,z) \, \overline{Q}_{\gamma,\beta}(g) \right)$$
$$-\log \left(\sum_{x' \in E, g \in I_{x'}} \prod_{(y \to z) \in g} (Q_{\gamma,\beta} Q_{\beta}^{-1})(y,z) \, \tilde{Q}_{\beta}(g) \right),$$

where

$$\overline{Q}_{\gamma,\beta}(g) = Q_{\gamma,\beta}(g) / \sum_{h \in I_x} Q_{\gamma,\beta}(h) \qquad \text{and} \qquad \tilde{Q}_{\beta}(g) = Q_{\beta}(g) / \sum_{z \in E, h \in I_z} Q_{\beta}(h).$$

By Jensen's inequality, we have

$$\log \frac{\pi_{\gamma,\beta}}{\pi_{\beta}}(x) \le 2 \sup_{g \in \cup_z I_z} |\log Q_{\gamma,\beta}(g) - \log Q_{\beta}(g)|.$$

Finally, we obtain

(20)
$$\operatorname{Ent}_{\pi_{\beta_t}}(m_t) \le \operatorname{Ent}_{\pi_{\gamma_t,\beta_t}}(m_t) + 2 \sup_{g \in \cup_x I_x} |\log Q_{\gamma_t,\beta_t}(g) - \log Q_{\beta_t}(g)|.$$

Using (9) the proof is complete.

We now make the above observations precise by considering more specific, although general, transitions $Q_{\gamma,\beta}$.

COROLLARY 4. Let V be a nonnegative function $V: E \times E \to \mathbb{R}_+$ and $Q_{\gamma,\beta}(x,y) = q_{\beta}(x,y) e^{\beta V_{\gamma}(x,y)}$. Suppose the assumptions of Corollary 2 are satisfied and, for every q(x,y) > 0,

(21)
$$|V_{\gamma_t}(x,y) - V(x,y)| = o(1/\log t).$$

When the inverse-freezing schedule has parametric form $\beta_t = K^{-1} \log t$, for t sufficiently large and K > c, we have

(22)
$$\lim_{t \to +\infty} Ent_{\pi_{\beta_t}}(m_t) = 0 \quad and \quad \lim_{t \to +\infty} P(X_t \in V^*) = 1,$$

where π_{β} is the unique invariant probability measure of the Markov generator $Q_{\beta} - I$ with

$$Q_{\beta}(x,y) = q(x,y) e^{-\beta V(x,y)}, \qquad V^* = \{x \in E : V(x) = \min_{E} V\},$$

and

$$V(x) = \min_{g \in G(x)} \sum_{(y \to z) \in g} V(y, z).$$

If $V_{\gamma_t}(x,y) = (U_t(y) - U_t(x))^+$ with $U_t : E \to \mathbb{R}_+$ and $\lim_{t \to +\infty} U_t(x) = U(x)$, condition (21) takes the form

$$\lim_{t \to +\infty} \log t |U_t(x) - U(x)| = 0.$$

The following examples illustrate the results and the conditions stated in the above theorems.

Examples.

1. Let us now turn our attention to the transition probability kernel

$$Q_{\gamma,\beta}(x,y) = q(x,y) e^{-\beta V_{\gamma}(x,y)},$$

where

$$V_{\gamma}(x,y) = (U_{\gamma}(y) - U_{\gamma}(x))^{+}$$
 if $q(x,y) > 0$ and $+\infty$ otherwise.

In this case conditions (6) and (7) take the form

$$\sup_{x \in E} U_{\gamma}(x) - \inf_{x \in E} U_{\gamma}(x) \le d_1(\gamma), \qquad \sup_{x \in E} \frac{d}{d\gamma} U_{\gamma}(x) - \inf_{x \in E} \frac{d}{d\gamma} U_{\gamma}(x) \le d_2(\beta)/\beta.$$

In addition, if

$$\sup_{x,\gamma} U_{\gamma}(x) < +\infty, \qquad \sup_{x,\gamma} \frac{d}{d\gamma} U_{\gamma}(x) < + infty,$$

then we can choose $d_2(\beta)=\beta\ d_2$ and $d_1(\gamma)=d_1<+\infty\ (d_1,d_2>0)$ and the condition (10) takes the form

$$\frac{d\gamma_t}{dt} = o(1/(t^{c/K}(\log t)^2)).$$

2. Let us examine the above example with time-inhomogeneous potential given by

$$U_{\gamma}(x) = \theta(\gamma)^{-1} \int_{0}^{\theta(\gamma)} C(s, x) ds$$

with $C: \mathbb{R}_+ \times E \to \mathbb{R}_+$ bounded and $\frac{d}{d\gamma} \log \theta(\gamma) < +\infty$.

From the boundedness of C we can choose constants $d_1, d_2 > 0$ so that $d_1(\gamma) = d_1$ and $d_2(\beta) = \beta d_2$ satisfy the required conditions. Finally, if $\gamma_t = A \log t$ and $\theta(\gamma) = e^{\gamma}$, then we have

$$\frac{d\gamma_t}{dt} = A/t = o\left(1/(t^{c/K}(\log t)^2)\right), \qquad \frac{d}{d\gamma}\log\theta(\gamma) = 1,$$

and

$$U_{\gamma_t}(x) = \frac{1}{t^A} \int_0^{t^A} C(s, x) \ ds.$$

1.2. General results on the virtual energy. In section 1 we proved the convergence in probability of a class of stochastic algorithms to the set of the global minima V^* of a virtual energy function V. The crucial need of course is to estimate V^* . In the case where q is symmetric and $V(x,y) = (U(y) - U(x))^+$ with $U: E \to \mathbb{R}_+$ it is well known that $V^* = U^*$. For a generalization of this see Trouvé [12]. The situation becomes considerably more involved when the above assumptions are dispensed with. The purpose of this section is to introduce a natural test set approach to study V^* . More precisely, we will give several conditions for a given subset $H \subset E$ to contain V^* .

Let us recall some basic definitions. Let E be a finite set and q an irreducible Markov kernel. Assume that a given function $V: E \times E \to \overline{\mathbb{R}}_+$ satisfies

$$V(x,y) < +\infty \iff q(x,y) > 0.$$

Let us write $C_{x,y}$ the paths p in E joining x and y, that is,

$$\forall k \in \{0, \dots, |p|-1\} \quad q(p_k, p_{k+1}) > 0 \quad \text{and} \quad p_0 = x, p_{|p|} = y,$$

where |p| is the length of p. For $x, y \in E$, $p \in C_{x,y}$, and $g \in G(x)$ we note

$$V(p) = \sum_{k=0}^{|p|-1} V(p_k, p_{k+1}), \qquad V(g) = \sum_{(y \to z) \in g} V(y, z), \qquad V(x) = \min_{g \in G(x)} V(g).$$

For $H \subset E$ and g an x-graph over H (that is, $g \in G_H(x)$) it is convenient to define a new communication cost V_H by making the set H a taboo set. Namely, for every $x, y \in H$

$$V_H(x,y) = \min \{ V(p) : p \in C_{x,y} \text{ with } \forall k \in \{1,\dots,|p|-1\} \ p_k \notin H \},$$
$$V_H(g) = \sum_{(y \to z) \in g} V_H(y,z).$$

It is also convenient to define the virtual energy function associated with V_H :

$$\forall x \in H \qquad V_H(x) = \min_{g \in G_H(x)} V_H(g) - \min_{y \in H, h \in G_H(y)} V_H(h).$$

Finally, let us write

$$V(H) = \min_{x \in H} V(x)$$
 and $V_H^{\star} = \left\{ x \in H : V_H(x) = \min_H V_H \right\}.$

LEMMA 2. $\forall x \in H, \ V_H(x) = V(x) - V(H).$

Lemma 2 is an easy consequence of the following lemma.

Lemma 3. Let Q be an irreducible transition probability over E with invariant measure μ . Let X be a Markov chain with transition probability Q and initial measure m such that $m(x) > 0 \ \forall x \in E$. Given a subset $H \subset E$ define

$$T_1 = \inf \{ n \ge 1 : X_n \in H \}$$
 $\tilde{Q} = P(X_{T_1} = y/X_0 = x).$

Then \tilde{Q} is an irreducible Markov kernel over H and its invariant probability measure is given by

$$\tilde{\mu}(x) = \mu(x)/\mu(H).$$

There are several ways to prove Lemmas 2 and 3. The following may be the shortest in this context.

Proof of Lemma 3. The proof is a consequence of the law of large numbers. Let us set by induction on the parameter $n \geq 1$

$$T_{n+1} = \inf \{ k > T_n : X_k \in H \}, \quad n \ge 1$$

Now, under the above conditions, the random process $Y = (Y_n)_{n \geq 0}$ defined by

$$Y_0 = X_0, Y_n = X_{T_n}, n \ge 1,$$

is an irreducible Markov chain over H with transition probability kernel \tilde{Q} . Let $\tilde{\mu}$ be its invariant probability measure. First we note that P-almost surely

$$\forall x \in E$$
 $\frac{1}{n} \sum_{i=1}^{n} 1_x(Y_i) \xrightarrow[n \to +\infty]{} \tilde{\mu}(x)$

On the other hand we have

$$\frac{1}{n}\sum_{i=1}^{n} 1_x(Y_i) = \frac{T_n}{n} \left(\frac{1}{T_n} \sum_{i=1}^{T_n} 1_x(X_i) \right), \qquad \frac{n}{T_n} = \frac{1}{T_n} \sum_{i=1}^{T_n} 1_H(X_i),$$

and

$$\frac{1}{T_n} \sum_{i=1}^{T_n} 1_x(X_i) \xrightarrow[n \to +\infty]{} \mu(x), \qquad \frac{1}{T_n} \sum_{i=1}^{T_n} 1_H(X_i) \xrightarrow[n \to +\infty]{} \mu(H)$$

P-almost everywhere (P.a.e.). The lemma follows immediately.

We come to the proof of Lemma 2.

Proof of Lemma 2. We shall give a sketch of the proof. Let us denote by Q_{β} the Markov kernel over E given by

$$Q_{\beta}(x,y) = \begin{cases} |E|^{-1} \exp{-\beta V(x,y)} & \text{if } x \neq y, \\ 1 - |E|^{-1} \sum_{z \in E: z \neq x} \exp{-\beta V(x,z)} & \text{otherwise.} \end{cases}$$

Let μ_{β} be the invariant measure of Q_{β} . From the description of μ_{β} in terms of x-graphs over E it is clear that

$$\mu_{\beta}(x) \sim C(x) \exp{-\beta V(x)}$$

for some nonnegative function $C: E \to \mathbb{R}_+^*$. If one now defines \tilde{Q}_{β} as in Lemma 3, by elementary large deviation arguments one sees the equivalence

$$\tilde{Q}_{\beta}(x,y) \sim \tilde{q}(x,y) \exp{-\beta V_H(x,y)} \quad \forall x, y \in H$$

for some irreducible Markov kernel $\tilde{q}: E \times E \to \mathbb{R}_+$. Therefore if $\tilde{\mu}_{\beta}$ is the invariant measure of \tilde{Q}_{β} one has for some nonnegative function $\tilde{C}: E \to \mathbb{R}_+^*$

$$\tilde{\mu}_{\beta}(x) \sim \tilde{C}(x) \exp{-\beta V_H(x)},$$

from which our claim follows easily.

We now give a definition that we will use in our formulation of our test set approach to understand the limiting behavior of a generalized simulated annealing.

DEFINITION 1. Let H be a subset of E. We say that a partition $\mathcal{H} = \{H_1, \ldots, H_n\}$ of H is a V-partition if for every $1 \leq i \leq n$ and $x, y \in H_i$, $x \neq y$, there exists a path $p \in C_{x,y}$ such that

$$\forall 0 \le k < |p| \qquad p_k \in H_i \quad and \quad V(p_k, p_{k+1}) = 0.$$

We observe that for a given subset $H \subset E$, one can always obtain a V-partition. For instance

$$\mathcal{H} = \{ \{x\} : x \in H \}$$

is a V-partition. Given a V-partition $\mathcal{H} = \{H_1, \ldots, H_n\}$ of $H \subset E$, it is convenient to define a new communication cost function $V_{\mathcal{H}}$ by setting for every $x \in H_i$ and $y \in H_j$, $1 \leq i, j \leq n$

$$V_{\mathcal{H}}(x,y) = \{ V(p) : p \in C_{x,y} \ \exists 0 \le n_1 < n_2 \le |p|$$
$$\forall 0 \le k \le n_1, p_k \in H_i, \ \forall n_1 < k < n_2, p_k \notin H, \ \forall n_2 \le k \le |p|p_k \in H_i \}.$$

It is easily seen that $V_{\mathcal{H}}(x,y)$ does not depend on the choice of $x \in H_i$ and $y \in H_j$. Moreover we note that if $\mathcal{H} = \{\{x\} : x \in H\}$, then $V_{\mathcal{H}} = V_H$.

Let $V_{\mathcal{H}}$ be the virtual energy function associated with the communication cost function $V_{\mathcal{H}}$, namely,

$$\forall x \in H \qquad V_{\mathcal{H}}(x) = \min_{g \in G_H(x)} V_{\mathcal{H}}(g) \qquad \text{with} \quad V_{\mathcal{H}}(g) = \sum_{(y \to z) \in g} V_{\mathcal{H}}(y, z).$$

As usual, we also put

$$V_{\mathcal{H}}^{\star} = \left\{ x \in H : V_{\mathcal{H}}(x) = \min_{H} V_{\mathcal{H}} \right\}.$$

PROPOSITION 2. If \mathcal{H} is a V-partition of a subset $H \subset E$, then we have $V_{\mathcal{H}} = V_H$.

Proof. Let us prove that for every $x \in H$

$$\min_{g \in G_H(x)} V_H(g) = \min_{g \in G_H(x)} V_H(g).$$

Because $\mathcal{H} = \{H_1, \ldots, H_n\}$ is a V-partition it is clear that $V_{\mathcal{H}} \leq V_H$. So our claim will follow provided that for every $g \in G_H(x)$ we can build a new $\tilde{g} \in G_H(x)$ such that $V_{\mathcal{H}}(g) \geq V_H(\tilde{g})$. For this purpose let $g \in G_H(x)$ for some $x \in H$ and let $i \in \{1, \ldots, n\}$ such that $x \in H_i$. We will construct an x-graph $\tilde{g} \in G_H(x)$ such that $V_{\mathcal{H}}(g) \geq V_H(\tilde{g})$. For this we introduce the set

$$\Gamma = \{(j \to k) : \exists (y, z) \in g \text{ such that } y \in H_j \text{ and } z \in H_k\}.$$

Obviously Γ is not an *i*-graph over $\{1,\ldots,n\}$ but examination of Γ soon yields that it contains at least one *i*-graph G_i . Now for $j \neq i$ and $(j \to k) \in G_i$ (unique) there exists an arrow $(y_j \to z_k) \in g$ such that $y_j \in H_j$ and $z_k \in H_k$.

On the other hand, from the definition of $V_{\mathcal{H}}$ there exists a path $p \in C_{y_j,z_k}$ and $0 \le n_1 < n_2 \le |p|$ such that

$$\forall 0 \le l \le n_1 \quad p_l \in H_i, \qquad \forall n_1 < l < n_2 \quad p_l \notin H, \qquad \forall n_2 \le l \le |p| \quad p_l \in H_k,$$

and $V(p) = V_{\mathcal{H}}(y_j, z_k)$. Given such a path $p \in C_{y_j, z_k}$ let us set

$$\tilde{y}_j = p_{n_1}, \qquad \tilde{z}_k = p_{n_2}.$$

Finally, because \mathcal{H} is a V-partition there exists for every $1 \leq i \leq n$ a \tilde{y}_j -graph $\tilde{g}_i \in G_{H_i}(\tilde{y}_i)$ such that $V(\tilde{g}_i) = 0$, with the convention $\tilde{y}_i = x$.

Using the above construction it is easily seen that the set of arrows

$$\tilde{g} = \bigcup_{i=1}^{n} \tilde{g}_{i} \bigcup_{(j \to k) \in G_{i}} \{ (\tilde{y}_{j} \to \tilde{z}_{k}) \}$$

is an x-graph over H and, from the construction of g, it follows that

$$V_{\mathcal{H}}(g) \ge V_{\mathcal{H}}(\tilde{g}) = \sum_{(j \to k) \in G_i} V_{\mathcal{H}}(\tilde{y}_j, \tilde{z}_k) = \sum_{(j \to k) \in G_i} V_{\mathcal{H}}(\tilde{y}_j, \tilde{z}_k) = V_{\mathcal{H}}(\tilde{g}).$$

This ends the proof.

The following concept of λ -stability leads to a natural test set approach to study V^* .

DEFINITION 2. Let λ be a nonnegative real number. A subset $H \subset E$ is called λ -stable with respect to a communication cost function V when the following conditions are satisfied:

- 1. $\forall x \in H \ \forall y \notin H, \qquad V(x,y) > \lambda,$
- 2. $\forall x \notin H \ \exists y \in H, \qquad V(x,y) < \lambda.$

The importance of the notion of λ -stability resides in the following result, which extends Lemma 4.1 of Freidlin–Wentzell [6].

Proposition 3. Let λ be a nonnegative real number and $H \subset E$. Any λ -stable subset H with respect to V contains V^* and $V_H = V_{/H}$

Proof. Let H be a λ -stable subset of E. Let $x \notin H$ and let g be an element of G(x) such that V(g) = V(x). There exists almost one $g \in H$ such that $V(x, y) \leq \lambda$. Now we note g the exit path from g to g extracted from g, that is,

$$p_0 = y, p_{|p|} = x$$
 and $\forall k = 0, \dots, |p| - 1, (p_k \to p_{k+1}) \in g.$

Write $k_0 = \inf\{k = 0, \dots, |p| - 1 : p_k \notin H\}$. Let \overline{g} be the graph obtained from g by replacing the arrow $(p_{k_0-1} \to p_{k_0})$ by $(x \to y)$. Then we have $\overline{g} \in G(p_{k_0-1})$ and

$$V(x) = V(g) > V(\overline{g}) \ge V(p_{k_0-1}), \quad p_{k_0-1} \in H.$$

This completes the proof of the first assertion. The last assertion is a clear consequence of Lemma 2. \Box

Let us now reduce all of the results of this section to a proposition which we shall use for later reference.

PROPOSITION 4. Let A be a 0-stable subset of E with respect to V and let A be a V-partition of A. If H is a λ -stable subset of A with respect to V_A for some $\lambda \geq 0$, then $V^* \subset H$.

Proof. Using Proposition 3 it is easily seen that $V^* \subset A$, $V_A = V_{/A} = V_{\mathcal{A}}$, and $V_{\mathcal{A}}^* \subset H$. Thus one gets $V^* = V_{\mathcal{A}}^* = V_{\mathcal{A}}^* \subset H$, and the proof of Proposition 4 is completed. \square

- 2. Applications. In this section we examine two applications. In section 2.1 we use the results of the first section to derive a new and simple proof of the convergence of the genetic algorithms. We shall prove this important result in a way different from the original proof of Cerf [2]. The proof splits quite naturally into two distinct parts:
 - 1. We use the relative entropy convergence results stated in the first section to prove the convergence of the algorithm.
 - 2. Then we investigate the test set approach, introduced in the second part of section 1, to prove that the set of the global minima of the virtual energy is contained in the product of the set of the global minima of the fitness function.

In section 2.2 we apply Corollary 4 to construct a stochastic algorithm for the numerical solving of a general mean cost optimization problem.

2.1. Genetic algorithms. A genetic algorithm is a discrete time Markov process $\hat{x} = (\hat{x}_n)_n$ with state space $E = S^N$ (N > 1 and S a finite set) and whose transition probabilities G_n include a mutation M_n and a selection S_n mechanism. The N-tuple of elements of S, i.e., the points of the set E, are called particle systems and most will be denoted by the letters x, y, z. In what follows, we shall distinguish two kinds of combinations, namely,

(a)
$$P\left(\widehat{x}_n \in dx / \widehat{x}_{n-1} = z\right) = \int_E M_n(z, dy) \, S_n(y, dx),$$

(b)
$$P(\hat{x}_n \in dx/\hat{x}_{n-1} = z) = \alpha M_n(z, dx) + (1 - \alpha) S_n(z, dx), \quad 0 < \alpha < 1.$$

Mutations. The mutation transition is modeled by independent motion of each particle, that is,

$$M_n(z, dy) = \prod_{p=1}^{N} K_n(z^p, dy^p),$$

where K_n is a Markov kernel over S, $z = (z^p)_{1 \le p \le N}$, and $y = (y^p)_{1 \le p \le N}$.

Selection. In the selection transition the particles are chosen randomly and independently in the previous population according to a given selection function $F_n: S \to \mathbb{R}^+$, namely,

$$S_n(y, dx) = \prod_{p=1}^N \sum_{i=1}^N \frac{F_n(y^i)}{\sum_{j=1}^N F_n(y^j)} 1_{y^i}(dx^p).$$

The study of the convergence, as $N \to +\infty$ or $n \to +\infty$, of such algorithms requires specific developments because each individual particle is no longer Markovian and it is difficult to produce mean error estimates. In [3] one of the authors applied and extended such algorithms to nonlinear filtering problems. An apparent difficulty in establishing a convergence result as $n \to +\infty$ is finding a candidate invariant measure that enables us to describe some aspects of the limiting behavior of the algorithm. To our knowledge, Cerf gives in his Ph.D. dissertation [2] the first convergence result $n \to +\infty$ for a genetic algorithm to converge in probability to the global minima of a given fitness function. More precisely, he studies the following situation:

- 1. The state space S is finite and $G_n = M_n S_n$.
- 2. The mutation Markov transition kernels $K_n(x^1, y^1)$ are governed by a parameter a and a cooling schedule $\beta(n) : \mathbb{N} \to \mathbb{R}^+$, namely,

(23)
$$M_n(x,y) = Q_{\beta(n)}^{(1)}(x,y) \stackrel{\text{def}}{=} \prod_{p=1}^N k_{\beta(n)}(x^p, y^p)$$

with

(24)
$$k_{\beta}(x^{1}, y^{1}) \stackrel{\text{def}}{=} \begin{cases} k(x^{1}, y^{1}) e^{-a \beta} & \text{if } x^{1} \neq y^{1}, \\ 1 - \sum_{z^{1} \neq x^{1}} k(x^{1}, z^{1}) e^{-a \beta} & \text{if } x^{1} = y^{1}, \end{cases}$$

where k is a given irreducible Markov kernel on the space S.

3. The selection operator is built with a fitness function $f: S \to \mathbb{R}^+$ and a cooling schedule $\beta(n): \mathbb{N} \to \mathbb{R}^+$, namely,

(25)
$$S_n(x,y) = Q_{\beta(n)}^{(2)}(x,y) \stackrel{\text{def}}{=} \prod_{p=1}^N \sum_{i=1}^N \frac{e^{-\beta(n) f(x^i)}}{\sum_{j=1}^N e^{-\beta(n) f(x^j)}} 1_{x^i}(y^p).$$

Cerf gives several conditions on the rate of decrease of the cooling schedule $\beta(n) \to +\infty$ to ensure all the particles visit the set of global minima, as times goes on, when the number of particles is greater than a critical value. He carries out in a discrete time setting a precise study using large deviation techniques and the powerful tools developed by Trouvé [12]. Simplifying and extending techniques of Cerf and Trouvé, our results are obtained by using the relative entropy convergence result stated in Corollary 1 and by investigating the test set approach introduced in section 1.2.

2.1.1. General results and notations. In this section we will consider genetic algorithms described by the transition probability kernel

$$Q_{\beta} = Q_{\beta}^{(1)} Q_{\beta}^{(2)}$$
 or $\tilde{Q}_{\beta} = \alpha_1 Q_{\beta}^{(1)} + \alpha_2 Q_{\beta}^{(2)}$ with $\alpha_1 + \alpha_2 = 1$ and $0 < \alpha_1 < 1$ (26)

and nonnecessarily vanishing mutations. More precisely, we assume that the mutation transition kernels k_{β} in (24) have the property

$$(27) \exists b > 0, \qquad b^{-1} \ k(x_1, x_2) \ e^{-\beta \ a(x_1, x_2)} \le k_{\beta}(x_1, x_2) \le b \ k(x_1, x_2) \ e^{-\beta \ a(x_1, x_2)},$$

where $a: S^2 \to \overline{\mathbb{R}}_+$, $a(x,y) < +\infty \iff k(x,y) > 0$, k is an irreducible Markov kernel, and the relation on S defined by

$$x_1 \sim x_2 \Longleftrightarrow a(x_1, x_2) = 0$$

is an equivalence relation. This leads us naturally to consider the partition $S_1, \ldots, S_{n(a)}$, $n(a) \geq 1$, induced by \sim . If x_1 is a typical element of S, then the equivalence class of x_1 will be denoted by $S(x_1)$:

$$S(x_1) = \{x_2 \in S : x_1 \sim x_2\}.$$

We further require that

$$a(x_1, x_2) = 0 \Longrightarrow f(x_1) = f(x_2)$$

and for some $\beta_0 > 0$

(28)
$$\forall x_1, x_2 \in S \qquad \sup_{\beta \ge \beta_0} |d \log k_\beta(x_1, x_2)/d\beta| < +\infty.$$

To our knowledge the models of evolutionary processes (26) have not been covered by the literature of genetic algorithms.

Examples. The following mutation transition kernels have the properties (27) and (28):

$$(28): \\ 1. \ k_{\beta}(x_{1}, x_{2}) = \begin{cases} k(x_{1}, x_{2}) \ e^{-\beta \ a(x_{1}, x_{2})} & \text{if} \quad a(x_{1}, x_{2}) > 0, \\ |S(x_{1})|^{-1} \left(1 - \sum_{y_{1} \notin S(x_{1})} \ k(x_{1}, y_{1}) \ e^{-\beta \ a(x_{1}, y_{1})} \right) & \text{otherwise.} \end{cases} \\ 2. \ k_{\beta}(x_{1}, x_{2}) = \frac{e^{-\beta \ a(x_{1}, x_{2})} \ k(x_{1}, x_{2})}{\sum_{y_{1} \in S} \ e^{-\beta \ a(x_{1}, y_{1})} \ k(x_{1}, y_{1})} \quad \forall (x_{1}, x_{2}) \in S^{2}. \end{cases}$$
 Finally, let us note that if a is given by

$$a(x_1, x_2) = a (1 - 1_{x_1}(x_2))$$
 $\forall (x_1, x_2) \in S^2 : k(x_1, x_2) > 0,$

then the first transition probability kernel is clearly the same as the mutation transition probability kernel (24) studied by Cerf.

In this special situation, the first model $Q_{\beta} = Q_{\beta}^{(1)} Q_{\beta}^{(2)}$ is of course identical to Cerf's model of a genetic algorithm.

Let us recall some terminology introduced by Cerf in [2]. The cardinality of a set will be denoted by |.|. If x and y belong to $E = S^N$ and $f: S \to \mathbb{R}^+$, we write

$$[x] = \{x_k : 1 \le k \le N\}, \qquad f^* = \{x_1 \in S : f(x_1) = \min_{S} f\},$$

$$\widehat{x} = \{k : 1 \le k \le N, f(x_k) = \widehat{f}(x)\}, \qquad \widehat{f}(x) = \min_{1 \le k \le N} f(x_k),$$

$$x(y_1) = \operatorname{Card}\{k : 1 \le k \le N, x_k = y_1\}.$$

Using these notations, an easy calculation shows that for k = 1 or k = 2

$$Q_{\beta}^{(k)}(x,y) = q_{\beta}^{(k)}(x,y) \; e^{-\beta V^{(k)}(x,y)}, \qquad q_{\beta}^{(k)}(x,y) = q^{(k)}(x,y) \; \theta_{\beta}^{(k)}(x,y),$$

where

$$q^{(1)}(x,y) = \prod_{i:a(x_i,y_j)>0} k(x_i,y_i), \qquad q^{(2)}(x,y) = \prod_{i=1}^N \frac{x(y_i)}{|\widehat{x}|},$$
$$V^{(1)}(x,y) = \sum_{i=1}^N a(x_i,y_i) \quad \text{if} \quad q^{(1)}(x,y) > 0,$$

$$V^{(2)}(x,y) = \sum_{i=1}^{N} \left(f(y_i) - \widehat{f}(x) \right) \quad \text{if} \quad q^{(2)}(x,y) > 0,$$

$$\theta_{\beta}^{(1)}(x,y) = \prod_{i:a(x_i,y_i)=0} k_{\beta}(x_i,y_i),$$

$$\theta_{\beta}^{(2)}(x,y) = \left(1 + |\widehat{x}|^{-1} \sum_{k \notin \widehat{x}} \exp{-\beta(f(x_k) - \widehat{f}(x))} \right)^{-N}.$$

As usual, we will use the convention

$$\forall k \in \{1, 2\} \qquad V^{(k)}(x, y) = +\infty \iff q^{(k)}(x, y) = 0.$$

The asymptotic mutation dynamics of the genetic algorithms is governed by the kernel k and the function a. The irreducibility condition on the kernel k and the fact that a is an equivalence relation are sufficient conditions to allow the system of particles to visit all the state space E. Thus, using the above notations, it is easily checked that

- $q^{(1)}$ is irreducible and $q^{(2)}(x,x) > 0$ for every $x \in E$;
- for every k = 1, 2 and $q^{(k)}(x, y) > 0$ we have $\sup_{\beta \geq \beta_0} |d \log \theta_{\beta}^k(x, y)/d\beta| < +\infty$ for some $\beta_0 \geq 0$.

Then, returning to our general model (12), the conditions introduced in Corollary 1 are satisfied in both situations:

1.
$$Q_{\beta}(x,y) \stackrel{\text{def}}{=} Q_{\beta}^{(1)} \ Q_{\beta}^{(2)}(x,y) = \sum_{u \in U} \overline{q}_{\beta}(x,u,y) e^{-\beta \overline{V}(x,u,y)}$$
 with $U = E, \overline{V}(x,u,y) = V^{(1)}(x,u) + V^{(2)}(u,y), \overline{q}(x,u,y) = q^{(1)}(x,u) q^{(2)}(u,y),$ and $\theta_{\beta}(x,u,y) = \theta_{\beta}^{(1)}(x,u) \theta_{\beta}^{(2)}(u,y), \overline{q}_{\beta}(x,u,y) = \theta_{\beta}(x,u,y) \overline{q}(x,u,y).$

2.
$$\tilde{Q}_{\beta}(x,y) \stackrel{\text{def}}{=} \alpha_{1} \ Q_{\beta}^{(1)}(x,y) + \alpha_{2} \ Q_{\beta}^{(2)}(x,y) = \sum_{u \in U} \overline{q}_{\beta}(x,u,y) e^{-\beta \overline{V}(x,u,y)}$$
 with $U = \{1,2\}, \overline{V}(x,u,y) = V^{(u)}(x,y), \overline{q}(x,u,y) = \alpha_{u} \ q^{(u)}(x,y),$ and $\theta_{\beta}(x,u,y) = \theta_{\beta}^{(u)}(x,y), \overline{q}_{\beta}(x,u,y) = \theta_{\beta}(x,u,y) \overline{q}(x,u,y).$

2.1.2. A convergence theorem. To clarify the notations, in the remainder of section 2 we will use the diacritic $(\tilde{\cdot})$ to distinguish the communication cost functions, the virtual energy function, and the critical height associated with the transition probability kernels Q_{β} from those associated with \tilde{Q}_{β} .

From the above observations and Corollary 1, choosing β of the form

$$\beta_t = K^{-1} \log t$$
, where $K > c$ (resp., $K > \tilde{c}$),

for t sufficiently large yields that the canonical process (Ω, P, F_t, X_t) associated with the family of generators $(L_{\beta_t})_{t\geq 0} = (Q_{\beta_t} - I)_{t\geq 0}$ (resp., $(\tilde{Q}_{\beta_t} - I)_{t\geq 0}$) converges in probability to the set of the global minima V^* (resp., \tilde{V}^*) of the virtual energy V (resp., \tilde{V}) associated with Q_{β} (resp., \tilde{Q}_{β}) and described in Corollary 1. One open problem is to compare c and \tilde{c} . Let us remark that \tilde{c} does not depend on the choice of the parameter $\alpha \in]0,1[$. In view of these observations the bulk of the proof rests on showing that V^* and \tilde{V}^* are subsets of (f^*) , where (f^*) is the set in E defined by

$$(f^{\star}) = \left\{ x \in E : \widehat{f}(x) = \min_{E} f \right\}.$$

The main purpose of this section is to prove a more general result. We will prove that V^* and \tilde{V}^* are subsets of $(f^*) \cap A$, where A is the set in E defined by

$$A = \{ x \in E : x_k \sim x_l \quad \forall 1 \le k, l \le N \}.$$

By A we will denote the partition of A induced by the equivalence relation \sim

$$A = \{A_1, \dots, A_{n(a)}\}, \qquad A_i = \{x \in E : [x] \subset S_i\} \qquad \forall 1 \le i \le n(a).$$

As usual we associate with each typical element $x = (x_1, \ldots, x_N) \in A$ the subset

$$A(x) = \{ y \in E : [y] \subset S(x_1) \}.$$

Note that A is 0-stable with respect to V and \tilde{V} . Moreover, from our constructions, a routine proof yields that A is a V and \tilde{V} -partition of A. In view of Propositions 2 and 3 it follows that $V^* \subset A$, $\tilde{V}^* \subset A$, and

$$\forall x \in A \qquad V(x) = \min_{g \in G_A(x)} V_{\mathcal{A}}(g), \qquad \tilde{V}(x) = \min_{g \in G_A(x)} \tilde{V}_{\mathcal{A}}(g).$$

Now, from Proposition 4, to prove that V^* and \tilde{V}^* are subsets of (f^*) it clearly suffices to find a constant λ such that the subset $(f^*) \cap A$ is λ -stable with respect to V_A and \tilde{V}_A .

As we will see such results hold when the size N of the particle systems is greater that a critical value which depends on the functions a and f. We shall study this critical size now, beginning with two important lemmas.

Before proceeding we need to introduce some additional notations.

By Γ_{x_1,x_2} , $x_1,x_2 \in S$, we denote the paths q in S joining x_1 and x_2 , that is,

$$\forall 0 \le l < |q|$$
 $k(x_l, x_{l+1}) > 0$, $q_0 = x_1$, $q_{|q|} = x_2$.

We will also denote R(a) as the smallest integer such that for every $x_1, x_2 \in S$ in two different classes there exists a path joining x_1 and x_2 with length $|q| \leq R(a)$. More precisely,

$$R(a) = \max_{1 \le i, j \le n(a)} \min_{(x_i, x_j) \in S_i \times S_j} \min_{q \in \Gamma_{x_i, x_j}} |q|.$$

It also will be convenient to use the following definitions:

LEMMA 4. For every $x, y \in A$ such that $\widehat{f}(x) \geq \widehat{f}(y)$ we have

(29)
$$\tilde{V}_{\mathcal{A}}(x,y) \le \delta(a) \ R(a).$$

Moreover, for every $x \in A$ there exists a state $y \in (f^*) \cap A$ such that

(30)
$$V_{\mathcal{A}}(x,y) \le (\delta(a) + \delta(f)) R(a).$$

LEMMA 5. For every $x, y \in A$ such that $\widehat{f}(x) < \widehat{f}(y)$ we have

(31)
$$V_{\mathcal{A}}(x,y) \ge \min(\Delta a, \Delta f) N \quad and \quad \tilde{V}_{\mathcal{A}}(x,y) \ge \min(\Delta a, \Delta f) N.$$

Let us write

$$\lambda(a,f) = (\delta(a) + \delta(f)) \ R(a), \qquad \tilde{\lambda}(a,f) = \delta(a) \ R(a),$$

$$N(a,f) = \lambda(a,f) / \min(\Delta a, \Delta f), \qquad \tilde{N}(a,f) = \tilde{\lambda}(a,f) / \min(\Delta a, \Delta f).$$

Combining Lemmas 4 and 5 one easily gets

$$N > N(a, f) \Longrightarrow (f^*) \cap A$$
 is $\lambda(a, f)$ -stable with respect to $V_{\mathcal{A}}$, $N > \tilde{N}(a, f) \Longrightarrow (f^*) \cap A$ is $\tilde{\lambda}(a, f)$ -stable with respect to $\tilde{V}_{\mathcal{A}}$.

These results and Proposition 4 combine to yield the following theorem.

THEOREM 3. We denote (Ω, P, F_t, X_t) as the canonical process associated with the family of generators $(L_{\beta_t})_{t\geq 0} = (Q_{\beta_t} - I)_{t\geq 0}$ (resp., $(\tilde{Q}_{\beta_t} - I)_{t\geq 0}$), c (resp., \tilde{c}) the critical height associated with the communication cost function V (resp., \tilde{V}), and m_t the distribution of X_t . If β_t assumes the parametric form $\beta_t = K^{-1} \log t$, for sufficiently large t, with K > c and if N > N(a, f) (resp., $\tilde{N}(a, f)$), then we have

$$\lim_{t \to +\infty} \operatorname{Ent}_{\pi_{\beta_t}}(m_t) = 0 \quad and \quad \lim_{t \to +\infty} P(X_t \in (f^*) \cap A) = 1,$$

where π_{β} is the invariant probability measure of $L_{\beta} = Q_{\beta} - I$ (resp., $\tilde{Q}_{\beta} - I$).

We come to the proof of Lemmas 4 and 5.

Proof of Lemma 4. Let $x = (x_1, \ldots, x_N)$ and $y = (y_1, \ldots, y_N)$ be two elements of A such that $\widehat{f}(x) \geq \widehat{f}(y)$. First let us remark that

$$x_1 \sim y_1 \Longrightarrow \forall 1 \le k \le N, \quad a(x_k, y_k) = 0 \Longrightarrow \forall 1 \le k \le N, \quad f(x_k) = f(y_k).$$

In this situation, a routine proof yields

$$V_{\mathcal{A}}(x,y) = 0$$
 and $\tilde{V}_{\mathcal{A}}(x,y) = 0$.

If $a(x_1, y_1) > 0$ then the irreducibility condition implies the existence of a path $q \in \Gamma_{x_1, y_1}$ and a pair of integers $0 \le n_1 < n_2 \le |q|$ such that

$$\forall 0 \le k \le n_1, \ q_k \in S(x_1), \quad \forall n_1 < k < n_2, \ q_k \notin S(x_1), \quad \forall n_2 \le k \le |q|, \ q_k \in S(y_1).$$
(32)

Let us prove (29). For this, let $p \in \tilde{C}_{x,y}$ be the path defined by

$$\forall 0 \le k \le |q|, \quad p_k = (q_k, x_2, \dots, x_N), \quad p_{|q|+1} = (y_1), \quad p_{|q|+2} = y.$$

From the definition of q we have

 $\forall 0 \le k \le n_1, \ p_k \in A(x), \quad \forall n_1 < k \le |q|, \ p_k \notin A, \quad \forall k \in \{|q|+1, |q|+2\}, \ p_k \in A(y).$ (33)

Moreover, it follows that

$$0 \le \sum_{k=0}^{n_1-1} \tilde{V}(p_k, p_{k+1}) \le \sum_{k=0}^{n_1-1} V^{(1)}(p_k, p_{k+1}) = 0,$$

$$0 \le \tilde{V}(p_{|q|}, p_{|q|+1}) \le V^{(2)}(p_{|q|}, p_{|q|+1}) = 0, \text{ and }$$

$$\tilde{V}(p_{|q|+1}, p_{|q|+2}) = V^{(1)}(p_{|q|+1}, p_{|q|+2}) = 0.$$

Now, it appears from the proceeding that

$$\tilde{V}(p) \leq \sum_{k=0}^{n_1-1} \tilde{V}(p_k, p_{k+1}) + \sum_{k=n_1}^{|q|-1} \tilde{V}(p_k, p_{k+1}) + \tilde{V}(p_{|q|}, p_{|q|+1}) + \tilde{V}(p_{|q|+1}, p_{|q|+2})$$

$$= \sum_{k=n_1}^{|q|-1} \tilde{V}(p_k, p_{k+1}) \leq \delta(a)|q|.$$

Therefore $\tilde{V}(x,y) \leq \delta(a) R(a)$ and the proof of (29) is completed.

The proof of (30) is just a little more complicated.

Suppose $x \in A$ and y' is an element of A such that $\widehat{f}(x) \geq \widehat{f}(y') = \min_S f$ and $a(x_1, y_1') > 0$. Let q be the path joining x_1 and y_1' and defined as in (32). Using the above notations, let $(t_m)_m$ be the sequence of integers defined by

$$t_0 = n_1, t_m = \inf \{ k > t_{m-1} : f(q_k) < f(q_{t_{m-1}}) \} \forall m \ge 1$$

Using the assumption $\widehat{f}(x) \geq \widehat{f}(y') = \min_S f$, examination of q soon yields that there exists an $m_0 \geq 1$ such that $t_{m_0} \leq n_2$ and $f(q_{t_{m_0}}) = \min_S f$. Consequently, we have constructed a sequence of states $(q_{t_m})_{0 \leq m \leq m_0}$ such that

(34)
$$\widehat{f}(x) = f(q_{t_0}) > f(q_{t_1}) > \dots > f(q_{t_m}) > \dots > f(q_{t_{m_0}}) = \widehat{f}(y),$$

where $y = (q_{t_{m_0}}, \dots, q_{t_{m_0}}) \in A \cap (f^*)$. With each state q_{t_m} we associate a state $p_m \in E, 0 \le m \le m_0$, by setting

$$p_{t_0} = (q_{t_0}, x_2, \dots, x_N), \qquad p_{t_m} = (q_{t_m}, \dots, q_{t_m}, x_N) \quad \forall 1 \le m \le m_0.$$

First we note that $p_{t_m} \not\in A \ \forall 1 \leq m \leq m_0$ and

$$\widehat{f}(x) = \widehat{f}(p_{t_0}) > \widehat{f}(p_{t_1}) > \dots > \widehat{f}(p_{t_m}) > \dots > \widehat{f}(p_{t_{m_0}}) = \min_{S} f = \widehat{f}(y).$$

Our next task is to construct a sequence of paths $(p^{(m)})_{0 \le m \le m_0+1}$ such that

$$p^{(0)} \in C_{x, p_{t_0}}, \quad p^{(m)} \in C_{p_{t_{m-1}}, p_{t_m}}, \quad \forall 1 \le m \le m_0 \quad p^{(m_0+1)} \in C_{p_{t_{m_0}}, y},$$

and

- the path $p^{(0)}$ has length $|p^{(0)}| = t_0$ and for every $0 \le k \le t_0$ the states $p_k^{(0)}$ belong to A(x);
- for every $1 \leq m \leq m_0$, $p^{(m)}$ is a path joining $p_{t_{m-1}}$ and p_{t_m} in time

$$|p^{(m)}| = t_m - t_{m-1},$$

and for every $0 \le k \le t_m - t_{m-1}$ the states $p_k^{(m)}$ do not belong to A except the first initial state $p_0^{(1)} = p_{t_0} \in A(x)$;

• $p^{(m_0+1)} = (p_{t_{m_0}}, y).$

It is straightforward to see that any path $p^{(0)}$ satisfying the above conditions has null cost, that is, $V(p^{(0)}) = 0$. Then, to obtain the desired upper bound it clearly suffices to have

$$\forall 1 \le m \le m_0$$
 $V(p^{(m)}) \le (t_m - t_{m-1}) (\delta(a) + \delta(f)).$

We proceed to define $(p^{(m)})_{0 \le m \le m_0+1}$ as follows:

1. In view of (32) and (34) it is natural to define the initial path $p^{(0)} \stackrel{\text{def}}{=} (p_0, \dots, p_{t_0})$ by setting

$$\forall 0 \le k \le t_0 = n_1$$
 $p_k = (q_k, x_2, \dots, x_N) \in A(x).$

As has already been noted, a simple calculation shows that

$$V(p^{(0)}) = \sum_{k=0}^{t_0-1} V^{(1)}(p_k, p_{k+1}) + V^{(2)}(p_{k+1}, p_{k+1}) = 0.$$

2. Taking into account that t_1 is the first time k such that $f(q_k) < \widehat{f}(x)$ we are lead to define $p^{(1)} \stackrel{\text{def}}{=} (p_{t_0}, p_{t_0+1}, \dots, p_{t_1})$ by setting

$$\forall t_0 \le k < t_1$$
 $p_k = (q_k, x_2, \dots, x_N),$ $p_{t_1} = (q_{t_1}, \dots, q_{t_1}, x_N).$

Let us write $\overline{p}_{t_1} = (q_{t_1}, x_2, \dots, x_N)$. In this situation $p_k \notin A \ \forall t_0 < k \leq t_1$ and it is easy to verify that

$$V(p^{(1)}) \leq \sum_{k=t_0}^{t_1-2} V^{(1)}(p_k, p_{k+1}) + V^{(2)}(p_{k+1}, p_{k+1}) + V^{(1)}(p_{t_1-1}, \overline{p}_{t_1})$$

$$+ V^{(2)}(\overline{p}_{t_1}, p_{t_1})$$

$$\leq (t_1 - t_0)(\delta(a) + \delta(f)).$$

3. As for item 2, we define the paths $p^{(m)} \stackrel{\text{def}}{=} (p_{t_{m-1}}, p_{t_{m-1}+1}, \dots, p_{t_m})$ for $2 \le m \le m_0$ by setting

$$\forall t_{m-1} \le k < t_m p_k = (q_k, q_{t_{m-1}}, \dots, q_{t_{m-1}}, x_N), \quad p_{t_m} = (q_{t_m}, \dots, q_{t_m}, x_N).$$

Here again we have $p_k \notin A \ \forall t_{m-1} \leq k \leq t_m$. Let us introduce a new state $\overline{p}_{t_m} = (q_{t_m}, q_{t_{m-1}}, \dots, q_{t_{m-1}}, x_N)$. It is then an elementary matter to prove the inequalities

$$\begin{split} V(p^{(m)}) & \leq \sum_{k=t_{m-1}}^{t_m-2} \left(V^{(1)}(p_k, p_{k+1}) + V^{(2)}(p_{k+1}, p_{k+1}) \right) \\ & + V^{(1)}(p_{t_m-1}, \overline{p}_{t_m}) + V^{(2)}(\overline{p}_{t_m}, p_{t_m}) \\ & \leq (t_m - t_{m-1} - 1) \; (\delta(a) + 2 \; \delta(f)) + \delta(a) + \delta(f) \\ & \leq (t_m - t_{m-1}) \; (\delta(a) + \delta(f)). \end{split}$$

4. Finally, let us note that

$$0 \le V(p^{(m_0+1)}) \le V^{(1)}(p_{t_{m_0}}, p_{t_{m_0}}) + V^{(2)}(p_{t_{m_0}}, y) = 0.$$

Consider the path $p = (p^{(0)}, \dots, p^{(m_0+1)}) \in C_{x,y}$ obtained by joining end to end all these paths. From the above inequalities it follows easily that $V(p) \leq |q|$ $(\delta(a) + \delta(f))$. As a clear consequence one gets

$$V_{\mathcal{A}}(x,y) \le (\delta(a) + \delta(f)) R(a).$$

This ends the proof of Lemma 4.

Much more is true. In view of our assumptions on the function a and the constructions given in the proof of Lemma 4 we observe easily that

$$\forall x \in A \qquad \forall y \in A \cap (f^*) \qquad V_{\mathcal{A}}(x,y) \le (\delta(a) + \delta(f)) \ R(a).$$

Proof of Lemma 5. Let (x,y) be a pair of points of A such that $\widehat{f}(x) < \widehat{f}(y)$. Now, let p belong to $\widetilde{C}_{x,y}$. Note that since $\widehat{f}(x) < \widehat{f}(y)$ there exists a real number λ such that $\widehat{f}(x) < \lambda < \widehat{f}(y)$. Let us set

$$\forall 0 \le l \le |q| \qquad I_l = \left\{ i \in \{1, \dots, N\} : f(p_l^i) > \lambda \right\} \quad \text{and} \quad n_l = |I_l|.$$

It follows easily that $n_0 = 0$ and $n_{|p|} = N$.

Now, let T_k , $0 \le k \le N$, be the first time $l \ge 0$ such that $n_l \ge k$. More precisely,

$$T_k = \inf \{ l \in \{0, \dots, |p|\} : n_l \ge k \} \quad \forall 0 \le k \le N.$$

Clearly it appears from the above that

(35)
$$T_0 = 0, T_N \le |p|, n_{T_N} = N, n_{T_0} = n_0 = 0.$$

By definition of the communication cost function $V^{(1)}$ we can see that

$$V^{(1)}(p_{T_k-1}, p_{T_k}) \ge \sum_{i \in I_{T_k} - I_{T_{k-1}}} a(p_{T_k-1}^i, p_{T_k}^i) \ge (n_{T_k} - n_{T_k-1}) \Delta a \qquad \forall 1 \le k \le N.$$

(36)

More precisely, p_{T_k-1} contains n_{T_k-1} individuals $p_{T_k-1}^i$ such that $f(p_{T_k-1}^i) > \lambda$ and p_{T_k} contains n_{T_k} individuals $p_{T_k}^j$ such that $f(p_{T_k}^j) > \lambda$. Therefore, if $V^{(1)}(p_{T_k-1}, p_{T_k}) < +\infty$, then the transition $p_{T_k-1} \to p_{T_k}$ necessarily involves at least $(n_{T_k} - n_{T_k-1})$ individual mutations.

Similarly, if $V^{(2)}(p_{T_k-1}, p_{T_k}) < +\infty$, then the system p_{T_k} contains at least $(n_{T_k} - n_{T_k-1})$ new individuals $p_{T_k}^i \in [p_{T_{k-1}}]$ such that $f(p_{T_k}^i) > \lambda$. Thus a discussion similar to that above leads to

(37)
$$V^{(2)}(p_{T_k-1}, p_{T_k}) \ge (n_{T_k} - n_{T_k-1}) \Delta f.$$

Finally, by definition of \tilde{V} , we have

$$\tilde{V}(q) \ge \tilde{V}(p_{T_1-1}, p_{T_1}) + \dots + \tilde{V}(p_{T_N-1}, p_{T_N}).$$

Let us remark that

$$n_{T_k-1} \le k-1 \le n_{T_{k-1}} \quad \forall 1 \le k \le N.$$

Thus, combining (36) and (37), we arrive at

$$\tilde{V}(q) \ge N \min(\Delta a, \Delta f).$$

Taking the minimum of all $p \in \tilde{C}_{x,y}$ and taking into account that $V \geq \tilde{V}$ we obtain

$$V(x,y) \ge \tilde{V}(x,y) \ge N \min(\Delta a, \Delta f).$$

Finally we have

$$\tilde{V}_{\mathcal{A}}(x,y) \geq \tilde{V}(x,y) \geq N \ \min{(\Delta a, \Delta f)} \ \ \text{and} \ \ V_{\mathcal{A}}(x,y) \geq V(x,y) \geq N \ \min{(\Delta a, \Delta f)}.$$

This ends the proof of Lemma 5. \square

П

Remark. Lemmas 4 and 5 show that the costs of good transitions are bounded whereas the costs of the bad ones increase at least linearly with the size of the system. On the basis of the definition of V and \tilde{V} and in view of the proof of these lemmas it is clear that the above result is easier to establish for the cost function \tilde{V} . It also turns out that the estimate of the cost of bad transitions with respect to \tilde{V} provides a quick and natural way to estimate their costs with respect to V.

In [2] an inductive proof of this result is presented for the genetic algorithm associated with V and without the equivalence relation considered here. The main contribution here is the extension of the results presented in [2] to any equivalence relation a and to the genetic algorithm associated with the cost function \tilde{V} .

On the other hand and in contrast to the inductive proof presented in [2], the approach described here is based on a precise study of the cost of bad or good paths.

The constants $\lambda(a, f)$, $\lambda(a, f)$ represent the difficulty for a population to travel from an equivalence class to better ones. In connection with this remark it is interesting to note that $\tilde{\lambda}(a, f)$ does not depend on the fitness function f and

$$\lambda(a, f) > \tilde{\lambda}(a, f).$$

In other words, it is more difficult for the genetic algorithm associated with V to move from one configuration to a better one. The above observations also imply that the critical value N(a, f) is greater than $\tilde{N}(a, f)$.

Examples. Let us see what happens when our second general model (26) is specialized for the case where the state is

$$S = \{-1, +1\}^{S}, \qquad S = [-n, n]^{p}, \qquad p \ge 1$$

and the fitness function $f: S \to \mathbb{R}$ is given by

$$f(x) = \frac{1}{2} \sum_{s \in S} \sum_{s' \in V_s} x(s) \ x(s') + \frac{1}{2} \sum_{s \in S} x(s),$$

where

$$\forall s \in \mathcal{S} \qquad V_s = \{ s' \in \mathcal{S} : |s_k - s'_k| \le 1, \ 1 \le k \le p \}.$$

Let k be the Markovian mutation kernel on S given by

$$k(x_1, x_2) = \frac{1}{|\mathcal{V}(x_1)|} \, 1_{\mathcal{V}(x_1)}(x_2),$$

$$\mathcal{V}(x_1) \stackrel{\text{def}}{=} \{ x_2 \in S : \operatorname{Card} \{ s \in \mathcal{S} : x_1(s) \neq x_2(s) \} \leq 1 \}.$$

Suppose that the function a is given by

$$a(x_1, x_2) = (1 - 1_{x_1}(x_2)) \quad \forall (x_1, x_2) \in S^2 : k(x_1, x_2) > 0.$$

Then, one can check that

$$R(a) \le \max_{x,y} \min_{q \in C_{x,y}} |q| = \operatorname{card}(S) = (2n+1)^p$$
 and $\delta(a) = \Delta(a) = 1$.

Let N be an integer that $N > (2n+1)^p$. The above theorem shows that N individuals will solve the optimization problem when using the genetic algorithm associated with \tilde{Q}_{β} .

2.2. Mean cost optimization. In this section we discuss the ways in which the results of section 1 are applied in mean cost optimization problems. Namely, the object will be to find the global minima of a function $V: E \to \mathbb{R}_+$ given by

$$V(x) = E(\mathcal{U}(Z,x)) \qquad \text{or} \qquad V(x) = \min_{g \in G(x)} \sum_{(y,z) \in g} E(\mathcal{V}(Z;y,z)),$$

where

- E is a finite set and G(x) is the set of x-graphs over E,
- Z is a random variable taking value in a finite set F (we denote μ its distribution),
- $U: F \times E \to \mathbb{R}_+$, and $\mathcal{V}: F \times E \times E \times \to \mathbb{R}_+$.

We have seen how to construct a stochastic algorithm converging in probability to global minima of the virtual energy associated with a communication cost function. It is clear from the description above that the appropriate communication cost function is given by

$$V(x,y) = (E(\mathcal{U}(Z;y)) - E(\mathcal{U}(Z;x)))^{+} \quad \text{or} \quad V(x,y) = E(\mathcal{V}(Z;y,z)).$$

Unfortunately the huge size of the set F often precludes the use of such an algorithm, and the essential problem is to compute a mean cost function at each step. Therefore it is natural to choose, for instance, a Markovian kernel K which ensures that

$$V_{\gamma_t}(x,y) = \frac{1}{t^A} \int_0^{t^A} \mathcal{V}(Z_s; x, y) \ ds \xrightarrow[t \to +\infty]{} V(x,y) = E(\mathcal{V}(Z; x, y)) \qquad \text{P.a.e.}$$

or
$$V_{\gamma_t}(x,y) = \left(\frac{1}{t^A} \int_0^{t^A} \mathcal{U}(Z_s;y) \, ds - \frac{1}{t^A} \int_0^{t^A} \mathcal{U}(Z_s;x) \, ds\right)^+$$

$$\xrightarrow[t \to +\infty]{} V(x,y) = \left(E(\mathcal{U}(Z;y)) - E(\mathcal{U}(Z;x))\right)^+ \quad \text{P.a.e.}$$

where

- $V_{\gamma} \stackrel{\text{def}}{=} 1/e^{\gamma} \int_{0}^{e^{\gamma}} \mathcal{V}(Z_{s}; x, y) \ ds \text{ or}$ • $V_{\gamma} \stackrel{\text{def}}{=} \left(\frac{1}{e^{\gamma}} \int_{0}^{e^{\gamma}} \mathcal{U}(Z_{s}; y) \ ds - \frac{1}{e^{\gamma}} \int_{0}^{e^{\gamma}} \mathcal{U}(Z_{s}; x) \ ds\right)^{+},$
- $\bullet \ \gamma_t = A \log t$
- Z_s is a time-homogeneous Markov process associated with the generator $\mathcal{L} = K I$.
- μ is an invariant measure of \mathcal{L} .

Before starting the description of our stochastic algorithm, we give some details about the above convergences.

LEMMA 6. Let K be a an irreducible transition kernel with unique invariant measure μ . For every $x, y \in E$ and A > 0 we have

$$\lim_{t \to +\infty} \sqrt{\frac{t^A}{\log t}} |V_{\gamma_t}(x, y) - V(x, y)| = 0 \qquad P.a.e.$$

Proof. In this situation it is well known that for every $x, y \in E$ there exists a bounded function F(.; x, y) such that

$$\mathcal{V}(.;x,y) - \mu(\mathcal{V}(.;x,y)) = \mathcal{L}(F(.;x,y))$$
 and $\mu(F(.;x,y) = 0.$

This equation is the Poisson equation associated with V(.; x, y) and \mathcal{L} . Thus, one gets the decomposition

$$\frac{1}{t} \int_0^t (\mathcal{V}(Z_s; x, y) - \mu(\mathcal{V}(.; x, y))) \ ds = \frac{1}{t} (F(Z_t; x, y) - F(Z_0; x, y) - M(x, y)_t),$$

where M(x,y) is a martingale with angle bracket $\langle M(x,y) \rangle$ given by

$$\langle M(x,y)\rangle_t = \sum_{z \in F} \int_0^t (F(z;x,y) - F(Z_s;x,y))^2 K(Z_s,z) ds.$$

Since the function F is bounded we have $\langle M(x,y)\rangle_t \leq c$ t for some nonnegative constant. Finally, by the standard iterated-log law and since jumps are bounded, it follows that

$$\frac{1}{t}M(x,y)_t \le \frac{\sqrt{2\,c\,t\log\log(c\,t)}}{t}$$

and thus $\lim_{t\to +\infty} \sqrt{\frac{t}{\log t}} \left| \frac{1}{t} M(x,y)_t \right| = 0$. This ends the proof.

Remark. The Poisson equation is a standard tool in the study of Markov processes. For instance it was also used by Younes [13] to study the convergence of a stochastic gradient algorithm to a maximum likelihood estimator. The context of Younes is more complex than those considered here, and the speed of convergence cannot be obtained by a mere application of the iterated logarithm law as before. But Younes also noticed that if the convergence is fast enough (in a negative power in time), then one can couple the estimation procedure to a simulated annealing algorithm (with the classical reversibility conditions) to get the global minima of a function depending on the parameter to be estimated. To do this, Younes uses the Dobrushin coefficients, but the entropy approach enables one to get more precise results on the admissible logarithmic schedules of temperature (the constant c given below).

Let us fix some terminology.

- Let $(\Omega^{(Z)}, P^{(Z)}, F_t^{(Z)}, Z_t)$ be the canonical process associated with the generator \mathcal{L} .
- For a given probability measure m on E, $\beta, \gamma \in C^1(\mathbb{R}_+, \mathbb{R}_+)$ and given the Markov process Z we note $(\Omega_{(Z)}, P_{(Z)}, F_{(Z),t}, X_t)$ the canonical process associated with the family of generators $(L_{\gamma_t,\beta_t})_{t\geq 0} = (Q_{\gamma_t,\beta_t} I)_{t\geq 0}$ whose initial condition is $m_0 = m$, and we note m_t the distribution of X_t , where

$$Q_{\gamma,\beta}(x,y) = q(x,y) e^{-\beta V_{\gamma}(x,y)}$$
 with q irreducible.

• To capture all randomness we note $\Omega = \Omega^{(Z)} \times \Omega_{(Z)}$, $F_t = F_t^{(Z)} \times F_{(Z),t}$, and we define P as follows:

$$\forall A \in F_{(Z),t} \in \qquad \forall B \in F_t^{(Z)} \qquad P(A \times B) = \int_B \ P_{(Z)}(A) \ dP^{(Z)}.$$

The above lemma and Corollary 4 lead us to the following proposition.

PROPOSITION 5. Let us set $c = \limsup_{\gamma \to +\infty} c(\gamma) < +\infty$ P.a.e., where $c(\gamma)$ is the critical height associated with the communication cost V_{γ} .

When the inverse-freezing schedule has parametric form $\beta_t = K^{-1} \log t$, for t sufficiently large and K > c, we have

(38)
$$\lim_{t \to +\infty} Ent_{\pi_{\beta_t}}(m_t) = 0 \quad P.a.e. \quad and \quad \lim_{t \to +\infty} P(X_t \in V^*) = 1,$$

where π_{β} is the unique invariant probability of $L_{\beta} = Q_{\beta} - I$ with

$$Q_{\beta}(x,y) = q(x,y) e^{-\beta V(x,y)}.$$

In many practical situations we also want a quantitative measure of the convergence (38). Unfortunately our method of proof is not suitable for estimating such quantitative behavior. In our settings a natural alternative approach is to look at the convergence of the mean value of the process $t \to \operatorname{Ent}_{\pi_{\beta_t}}(m_t)$ with respect to the random media (given by Z). In view of the inequality (20) we immediately observe that the speed of convergence of the mean value is related to the speed of convergence of the mean values of $\operatorname{Ent}_{\pi_{\gamma_t,\beta_t}}(m_t)$ and $|V_{\gamma_t}(x,y)-V(x,y)|$. The first term, linked to the critical height $c(\gamma_t)$ and to the derivative of γ_t , depends in a complicated way on the constant A, but we know that it is a nondecreasing function of the parameter A. On the other hand, the second term is a nonincreasing function of the parameter A. If we know how these quantities are linked to A a good adjustment of this parameter is then related to a classical minimization problem. We will examine this quantitative behavior in a forthcoming paper.

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