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THE FREE ENERGY METHOD FOR THE FOKKER-PLANCK EQUATION OF THE WRIGHT-FISHER MODEL

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Abstract. We use the free energy functional associated with the Fokker-Planck (forward Kolmogorov) equation to investigate the convergence to equilibrium of the Wright-Fisher model of population genetics in the case of positive mutation rates.

Contents

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1. Introduction

In this paper, we shall systematically construct free energy functionals for the Kolmogorov forward equations (Fokker-Planck equations) for the Wright-Fisher model of population genetics with mutation and possibly also selection (see [10]). We shall then use them to construct a necessary and sufficient condition for the Wright-Fisher diffusion processes to have a unique stationary reversible probability measure. When this condition is satisfied, we show that the flow of probability measures (densities) exponentially converges to the stationary reversible one under various notions of distance (total variation, entropy, L^1, etc.).

The stationary distribution is an important quantity in conservative Markov processes. These processes include the diffusion processes derived from population genetics. However, in general it is not so easy to get the explicit form of a stationary distribution. A more tractable but much stronger condition is reversibility. Reversibility means that at stationarity the process has the same distribution as its time reversal. Typically, stationary distributions that can be computed explicitly turn out to be also reversible. In population genetics, reversibility concerns

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the prospective and retrospective aspects of the process; this is discussed in [10] p.107. See also, for example, [21], [24], [28] for various applications of reversibility in population genetics models.

For jump processes, the reversibility condition for a distribution μ can be usually localized and one gets equalities connecting jump rates with point masses (if μ is Gibbsian, this type of equalities is called the condition of detailed balance in the physics literature). For diffusion processes, such a localization is just integration by parts, and conditions for existence of a reversible distribution have been studied in great detail (see, for example, [18]).

In [29], Wright found a sufficient condition for a Wright-Fisher model with general mutation rates to have a unique stationary distribution. The sufficient condition for the Wright-Fisher model of 2 alleles with mutation and selection was also proved by Ethier and Kurtz ([9], p. 417). These sufficient conditions are the positivity and the uniformness of mutations (i.e. mutations depend only on the target alleles or independent parent; this is automatically satisfied in the case of 2 alleles). This then leads to question whether these conditions are also necessary. This kind of question has also been asked in more general models such as Fleming-Viot models and the answer is affirmative. In [22], a necessary and sufficient condition for the Fleming-Viot process with mutation, selection to be reversible is studied by using moment calculations. In [14], a necessary and sufficient condition for the Fleming-Viot process with mutation, selection and recombination to be reversible is studied by using quasi-invariant measures with a cocycle. In this paper, by using the free energy functional method, we show that the uniformness of mutations is the necessary and sufficient condition for the Wright-Fisher model with general mutation and selection to have a unique stationary reversible distribution.

The evolution of many physical or biological systems is driven by the interplay between diffusion and drift mechanisms. In particular, the competition between them may lead the system to a thermodynamical equilibrium. A currently very active research direction consists in studying the rate of convergence to equilibrium for a class of such Fokker Planck type equations (see, for example, [1], [5] for spatially homogeneous systems, [7], [15], [8] for spatially inhomogeneous systems). In particular, the connection between the convergence to equilibrium for the Fokker-Planck equations and inequalities from functional analysis, like logarithmic Sobolev, spectral gap, curvature-dimension has been recently actively studied (see, for example, [2], [23], [6], [3]). Here, we shall use such techniques to consider the rate of convergence to the stationary reversible distribution for Wright-Fisher diffusion models. The difference and also difficulty is that our state space is a non-smooth manifold (simplex) and the diffusion coefficients of the Fokker Planck operator are singular, i.e., they vanish on the boundary.

The rest of this paper is organized as follows. In Section 2, after some preliminaries, we obtain the first main result of a necessary and sufficient condition to have a unique stationary reversible density (Theorem 2.10). In Section 3, we systematically construct free energy functionals for the Wright-Fisher diffusion process with general mutation and selection. Combining this with Theorem 2.10, we prove that the necessary and sufficient condition for the existence of a unique stationary reversible distribution is that mutations are uniform (Theorems 3.2, 3.3). In Section 4, we shall consider the evolution of the free energy functional constructed in Section 3 in the case of uniform mutations (to guarantee that there exists a unique stationary reversible distribution). We shall prove that the difference of the current and the final (minimal/Gibbs) free energy is nothing but the relate entropy of the corresponding densities (Theorem 4.6) and the rate of change of this difference is the negative of the entropy production (also called Fisher information in the terminology of information geometry) (Theorem 4.7). In Section 5, under some conditions on the mutation coefficients, we shall show that the current distribution will converge in various senses to the stationary distribution, which is a Gibbs distribution (a distribution of the type of an exponential family in the terminology of information geometry) (Theorem 5.12, and Corollaries 5.15, 5.13, 5.14).

2. Preliminaries

We begin with some general concepts in order to introduce the theoretical context; a good reference is [3]. In this paper, we denote by Ω a Polish space (complete metric and separable).

Definition 2.1. A probability measure μ on Ω is called *stationary (invariant)* with respect to the (Markov) diffusion process $\mathbf{X}_t$ with semigroup $(T_t)_{t\geq 0}$ on Ω and generator $\mathcal{L}_n$ if

$$\int_\Omega T_t f(\mathbf{x})\mu(d\mathbf{x}) = \int_\Omega f(\mathbf{x})\mu(d\mathbf{x}), \quad \forall t \geq 0, f \in C_0^\infty(\Omega), \tag{2.1}$$

or equivalently (due to [11] Theorem 2.3)

$$\int_\Omega \mathcal{L}_n f(\mathbf{x})\mu(d\mathbf{x}) = 0, \quad \forall f \in C_0^\infty(\Omega). \tag{2.2}$$

It is called *reversible* if

$$\int_\Omega g(\mathbf{x}) T_t f(\mathbf{x})\mu(d\mathbf{x}) = \int_\Omega f(\mathbf{x}) T_t g(\mathbf{x})\mu(d\mathbf{x}), \quad \forall t \geq 0, f, g \in C_0^\infty(\Omega), \tag{2.3}$$

or equivalently

$$\int_\Omega g(\mathbf{x}) \mathcal{L}_n f(\mathbf{x})\mu(d\mathbf{x}) = \int_\Omega f(\mathbf{x}) \mathcal{L}_n g(\mathbf{x})\mu(d\mathbf{x}), \quad \forall f, g \in C_0^\infty(\Omega). \tag{2.4}$$

Definition 2.2. For a nonnegative functional $f(\mathbf{x})$ defined on a $\sigma-$finite measure space (Ω, μ), we define its (negative) entropy functional by

$$S_\mu(f) := \int_\Omega f \log f d\mu - \Big(\int_\Omega f d\mu \Big) \log \Big(\int_\Omega f d\mu \Big). \tag{2.5}$$

If $f(\mathbf{x})$ is a density with respect to μ, i.e. $\int_\Omega f d\mu = 1$ then this reduces to the standard negative entropy functional,

$$S_\mu(f) = \int_\Omega f \log f d\mu. \tag{2.6}$$

Definition 2.3. We say that the family of densities $\{u(\cdot, t)\}_{t\geq 0}$ on a $\sigma-$finite measure space (Ω, μ) satisfies the condition $I(A, \psi)$ if it solves a diffusion equation of the form

$$\begin{aligned} \partial_t u(\mathbf{x}, t) &= \partial_i \Big(A^{ij}(\mathbf{x}) \partial_j u(\mathbf{x}, t) + A^{ij}(\mathbf{x}) u(\mathbf{x}, t) \partial_j \psi(\mathbf{x}) \Big) \\ &= \nabla_\mathbf{x} \cdot \Big(A(\mathbf{x}) \nabla_\mathbf{x} u(\mathbf{x}, t) + A(\mathbf{x}) u(\mathbf{x}, t) \nabla \psi(\mathbf{x}) \Big) \\ &= \nabla_\mathbf{x} \cdot \Big(A(\mathbf{x}) u(\mathbf{x}, t) \nabla_\mathbf{x} \big(\log u(\mathbf{x}, t) + \psi(\mathbf{x}) \big) \Big), \end{aligned} \tag{2.7}$$

where

$$A^{ij}(\mathbf{x}) = A^{ji}(\mathbf{x}),$$

and it satisfies the condition $II(A, \psi)$ if in addition to $I(A, \psi)$, ψ, we also have

$$\int_\Omega e^{-\psi(\mathbf{x})} \mu(d\mathbf{x}) < \infty.$$

Definition 2.4. For a family of densities $\{u(\cdot,t)\}_{t\geq 0}$ on a $\sigma-$finite measure space (Ω,μ) with condition $I(A,\psi)$, we define the potential energy functional by

$$\Psi(u(\cdot,t)) := \int\limits_{\Omega} u(\mathbf{x},t)\psi(\mathbf{x})\mu(d\mathbf{x}). \tag{2.8}$$

and the free energy functional by

$$\begin{aligned} F(u(\cdot,t)) &:= \int\limits_{\Omega} u(\mathbf{x},t)\Big(\log u(\mathbf{x},t)+\psi(\mathbf{x})\Big)\mu(d\mathbf{x}) \\ &= S_\mu(u(\cdot,t)) + \Psi(u(\cdot,t)). \end{aligned} \tag{2.9}$$

We can extend this functional to the space of all densities $\mathcal{D}$ as

$$F_\psi(q) := \int\limits_{\Omega} q(\mathbf{x})\Big(\log q(\mathbf{x})+\psi(\mathbf{x})\Big)\mu(d\mathbf{x}) \tag{2.10}$$

Remark 2.5. In the important paper [19], the relation between a Fokker-Planck equation and the associated free energy functional was systematically explored. In particular, it was demonstrated that a Fokker-Planck equation with gradient drift term may be interpreted as a gradient flux, or a steepest descent, of a free energy functional with respect to a certain (Wasserstein) metric.

Definition 2.6. Let f_1, f_2 be densities on a $\sigma-$finite measure space (Ω,μ). The relative entropy (Kullback–Leibler divergence) of f_1 with respect to f_2 is

$$D_{\mathrm{KL}}(f_1\|f_2) := \begin{cases} \int_\Omega f_1(\mathbf{x})\log\frac{f_1(\mathbf{x})}{f_2(\mathbf{x})}\mu(d\mathbf{x}), & \text{if } \mathrm{supp(f_1)}\subset \mathrm{supp(f_2)} \\ \infty, \ \text{otherwise} \end{cases}$$

Definition 2.7. The measure μ satisfies the logarithmic Sobolev inequality $LSI(\rho)$ (see also [13]) if for all densities f we have

$$\int_\Omega f\log f d\mu \leq \frac{1}{\rho}\int_\Omega \frac{1}{2f}|\nabla f|^2 d\mu.$$

Definition 2.8. The measure μ satisfies the spectral gap condition $SG(\rho)$ if for all functions h with $\int_\Omega h(x)\mu(dx)=0$, we have

$$\int_\Omega h^2 d\mu \leq \frac{1}{\rho}\int_\Omega |\nabla h|^2 d\mu.$$

Definition 2.9. A family of densities $\{u(\cdot,t)\}_{t\geq 0}$ on a $\sigma-$finite measure space (Ω,μ) is called hypercontractive with respect to μ if for all p_t satisfying

$$p_t - 1 = e^{2\rho t}(p_0-1),$$

we have

$$\left(\int_\Omega \big|u(x,t)\big|^{p_t} d\mu(x)\right)^{\frac{1}{p_t}} \leq \left(\int_\Omega \big|u(x,0)\big|^{p_0} d\mu(x)\right)^{\frac{1}{p_0}}.$$

Theorem 2.10. *The condition $II(A,\psi)$ is necessary and sufficient for the existence of a unique stationary reversible density.*

Proof. $\Rightarrow$: We assume that $\{u(\cdot,t)\}_{t\geq 0}$ satisfies the condition $II(A,\psi)$, i.e. $\partial_t u = Lu$ with

$$Lu = \nabla\cdot(A(\mathbf{x})\nabla u) + \nabla\cdot(A(\mathbf{x})u\nabla\psi(\mathbf{x})),$$

where $\psi(\mathbf{x})$ satisfies

$$\int_\Omega e^{-\psi(\mathbf{x})}d\mathbf{x} < \infty. \tag{2.11}$$

Then the generator L^* is of the form

$$L^* f = \nabla\cdot(A(\mathbf{x})\nabla f) - A(\mathbf{x})\nabla\psi(\mathbf{x})\cdot\nabla f \tag{2.12}$$

By (2.11), $\mu_\infty(d\mathbf{x}) = \frac{e^{-\psi(\mathbf{x})}}{Z}d\mathbf{x}$ is well-defined. By Lemma 4.5 below, $\mu_\infty(d\mathbf{x}) = \frac{e^{-\psi(\mathbf{x})}}{Z}d\mathbf{x}$ is reversible with respect to L^*. Then $\mu_\infty(d\mathbf{x}) = \frac{e^{-\psi(\mathbf{x})}}{Z}d\mathbf{x}$ is also stationary with respect to L^*, by applying the reversibility condition, which we have just observed, with an arbitrary f and $g=1$ and using $L^*1 = 0$.

We now want to show that $\mu_\infty(d\mathbf{x}) = \frac{e^{-\psi(\mathbf{x})}}{Z}d\mathbf{x}$ is the unique absolutely continuous stationary density reversible with respect to L^*. Thus, assume that ν is absolutely continuous, stationary and reversible with respect to L^*. Then $\nu(d\mathbf{x}) = k(\mathbf{x})\mu_\infty(d\mathbf{x})$ for some positive function k and of course we also have $\mu_\infty(d\mathbf{x}) = k(\mathbf{x})^{-1}\nu(d\mathbf{x})$. Therefore

$$\begin{aligned} 0 &= \int_\Omega L^* f d\nu \\ &= \int_\Omega L^* f k d\mu_\infty \\ &= \int_\Omega f L^* k d\mu_\infty, \qquad \text{due to the symmetry of } \mu_\infty \end{aligned} \tag{2.13}$$

This implies that $L^*k = 0$. Similarly, because of the symmetry of ν, we also have $L^*(k^{-1}) = 0$. Thus

$$\begin{aligned} 0 &= L^*(1) - kL^*(k^{-1}) - k^{-1}L^*k \\ &= A^{ij}(\mathbf{x})\partial_i k\partial_j k^{-1} \\ &= -\frac{A^{ij}(\mathbf{x})\partial_i k\partial_j k}{k^2} \end{aligned} \tag{2.14}$$

which implies that k is constant. Because ν and μ_∞ are probability measures, $k=1$. This means that $\nu = \mu_\infty$, which is the desired uniqueness.

$\Leftarrow$: Assume that $\nu(d\mathbf{x}) = v(\mathbf{x})d\mathbf{x}$ is an absolute continuous stationary probability measure that is reversible with respect to L^*. This implies that $Lv = 0$, where

$$Lv = \nabla\cdot(A(\mathbf{x})\nabla v) + \nabla\cdot(A(\mathbf{x})vZ(\mathbf{x}))$$

for some vector Z depending on $b^i(\mathbf{x})$ and $A^{ij}(\mathbf{x})$. Solving it we have

$$\nabla\log v = -Z(\mathbf{x}).$$

Thus, Z is of the form $\nabla\psi$ for some ψ. Thus, $v = Ce^{-\psi}$. Because of $\int_\Omega v d\mathbf{x} = 1$ we obtain $C = \frac{1}{Z} < \infty$, which means that $\{u(\cdot,t)_{t\geq 0}\}$ satisfies the condition $II(A,\psi)$. This completes the proof.

∎

3. The free energy of Wright–Fisher models

3.1. **Mutation only.** For reasons of exposition, we first present the case where there is no selection. In fact, as we shall see below, selection can be easily incorporated, because in contrast to mutation, it does not produce any potential singularities. Selection, however, introduces additional terms that make the notation more complicated without touching the essence of the mathematics.

For a diploid Wright Fisher population of N individuals with $n+1$ alleles $A^0, \dots, A^n$ undergoing mutations from A^i to A^j with rates $\frac{\theta_{ij}}{4N} \in \mathbb{R}$ for all $i \neq j \in \{0, 1, \cdots, n\}$, the expectation values for the change of the relative frequencies $\mathbf{X}_t = (X_t^1, \dots, X_t^n)$ of the alleles $(A^1, \dots, A^n)$ and $X_t^0 = 1 - X_t^1 - \cdots - X_t^n$ for allele A^0 at generation $2Nt$ satisfy (see, for instance, [10])

$$
\begin{aligned}
\mathbb{E}(\delta X_t^i | \mathbf{X}_t) &= b^i(\mathbf{X}_t)(\delta t) + o(\delta t); \\
\mathbb{E}(\delta X_t^i \delta X_t^j | \mathbf{X}_t) &= a^{ij}(\mathbf{X}_t)(\delta t) + o(\delta t), \quad \forall i, j = 1, \dots, n; \\
\mathbb{E}((\delta \mathbf{X}_t)^{\boldsymbol{\alpha}} | \mathbf{X}_t) &= o(\delta t), \quad \text{for } |\boldsymbol{\alpha}| \geq 3,
\end{aligned}
\tag{3.1}
$$

with the drift term

$$b^i(\mathbf{x}) = -\Big(\sum_{j=0}^n \frac{1}{2}\theta_{ij}\Big)x^i + \sum_{j=0}^n \frac{1}{2}\theta_{ji}x^j, \quad i = 1, \dots, n;$$

and the diffusion term

$$a^{ij}(\mathbf{x}) = x^i(\delta_{ij} - x^j) \quad i, j = 1, \dots, n.$$

Remark 3.1. Putting

$$b^0(\mathbf{x}) = -\frac{1}{2}\Big(\sum_{j=0}^n \theta_{0j}\Big)x^0 + \frac{1}{2}\sum_{j=0}^n \theta_{j0}x^j$$

we have

$$\sum_{i=0}^n b^i(\mathbf{x}) = 0.$$

We shall prove that

Theorem 3.2. *In a diploid Wright–Fisher model of N individuals with $n+1$ alleles with general mutation rates, a necessary and sufficiency condition to have a unique stationary distribution is*

$$\theta_{ij} = \theta_j > 0 \quad \textit{for all } i \neq j, \quad i, j = 0, \dots, n. \tag{3.2}$$

The stationary distribution in this case is of the form

$$\mu_\infty^m(d\mathbf{x}) = f_\infty^m(\mathbf{x})d\mathbf{x} = \frac{e^{-\psi(\mathbf{x})}}{Z(\boldsymbol{\theta})}d\mathbf{x} = \frac{\Pi_{i=0}^n (x^i)^{\theta_i - 1}}{Z(\boldsymbol{\theta})}d\mathbf{x}. \tag{3.3}$$

Proof. Again, we consider the Kolmogorov forward equation for the density function $u(\mathbf{x}, t)$

$$\partial_t u(\mathbf{x}, t) = \sum_{i,j=1}^n \frac{\partial^2}{\partial x^i \partial x^j}\Big(\frac{a^{ij}(\mathbf{x})}{2}u(\mathbf{x}, t)\Big) - \sum_{i=1}^n \frac{\partial}{\partial x^i}\Big(b^i(\mathbf{x})u(\mathbf{x}, t)\Big). \tag{3.4}$$

To use the free energy method, we rewrite this equation in divergence form:

$$\begin{aligned}
\partial_t u(\mathbf{x},t) &= \sum_{i=1}^n \frac{\partial}{\partial x^i}\left(\sum_{j=1}^n \frac{\partial}{\partial x^j}\Big(\frac{a^{ij}(\mathbf{x})}{2}u(\mathbf{x},t)\Big)\right) - \sum_{i=1}^n \frac{\partial}{\partial x^i}\Big(b^i(\mathbf{x})u(\mathbf{x},t)\Big)\\
&= \sum_{i=1}^n \frac{\partial}{\partial x^i}\left(\sum_{j=1}^n \Big(A^{ij}(\mathbf{x})\frac{\partial}{\partial x^j}u(\mathbf{x},t)\Big)\right) + \sum_{i=1}^n \frac{\partial}{\partial x^i}\left(\Big(\sum_{j=1}^n \frac{\partial}{\partial x^j}A^{ij}(\mathbf{x}) - b^i(\mathbf{x})\Big)u(\mathbf{x},t)\right)\\
&= \sum_{i=1}^n \frac{\partial}{\partial x^i}\left(\sum_{j=1}^n \Big(A^{ij}(\mathbf{x})\frac{\partial}{\partial x^j}u(\mathbf{x},t)\Big)\right) + \sum_{i=1}^n \frac{\partial}{\partial x^i}\left(\Big(\frac{1-(n+1)x^i}{2} - b^i(\mathbf{x})\Big)u(\mathbf{x},t)\right)\\
&= \nabla\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t)) + \nabla\cdot(A(\mathbf{x})u(\mathbf{x},t)\nabla\psi(\mathbf{x})),
\end{aligned} \tag{3.5}$$

with the gradient

$$\nabla = \Big(\frac{\partial}{\partial x^1},\dots,\frac{\partial}{\partial x^n}\Big)$$

and the diffusion coefficients

$$A(\mathbf{x}) = \Big(A^{ij}(\mathbf{x})\Big)_{i,j=1}^n = \frac{1}{2}\Big(a^{ij}(\mathbf{x})\Big)_{i,j=1}^n.$$

ψ then has to satisfy

$$\Big(A(\mathbf{x})\nabla\psi(\mathbf{x})\Big)_i = \frac{1-(n+1)x^i}{2} - b^i(\mathbf{x})$$

and hence

$$\begin{aligned}
\partial_i\psi(\mathbf{x}) &= \sum_{j=1}^n 2\left(\frac{\delta_{ij}}{x^j} + \frac{1}{x^0}\right)\left(\frac{1-(n+1)x^j}{2} - b^j(\mathbf{x})\right)\\
&= \frac{1-2b^i(\mathbf{x})}{x^i} - \frac{1-2b^0(\mathbf{x})}{x^0}\\
&= f_i(\mathbf{x}) - f_0(\mathbf{x}).
\end{aligned} \tag{3.6}$$

We are looking for conditions for the rates θ_{ij} so that there is a potential function.

Such a ψ exists if and only if (see [16] page 253)

$$\partial_j\Big(f_i(\mathbf{x}) - f_0(\mathbf{x})\Big) = \partial_i\Big(f_j(\mathbf{x}) - f_0(\mathbf{x})\Big).$$

This is equivalent to

$$-\frac{\theta_{ji}}{x^i} + \frac{\theta_{0i}}{x^i} + \frac{\theta_{j0}}{x^0} = -\frac{\theta_{ij}}{x^j} + \frac{\theta_{0j}}{x^j} + \frac{\theta_{i0}}{x^0}, \quad \forall i\neq j, \mathbf{x}\in int\Delta_n.$$

Here, Δ_n is the probability simplex $\{\mathbf{x} = (x^0,\dots,x^n) : x^i \geq 0, \sum_j x^j = 1\}$. Letting $x^i \to 0$ while keeping x^j, x^0 fixed, we conclude that $\theta_{ji} = \theta_{0i}$ for all $j \neq i$. Similarly, we obtain $\theta_{ij} = \theta_{0j}$ and $\theta_{j0} = \theta_{i0}$. It follows that

$$\theta_{ij} = \theta_j \quad \text{for all } i\neq j, \quad i,j = 0,\dots,n. \tag{3.7}$$

From (3.6), we then get

$$\psi(\mathbf{x}) = \sum_{i=0}^n (1-\theta_i)\log(x^i).$$

Moreover, ψ then satisfies

$$\int_{\Delta_n} e^{-\psi(\mathbf{x})} d\mathbf{x} < \infty$$

if and only if $\theta_i > 0$ for all i. □

For a diploid Wright–Fisher population with uniform mutation rates $\frac{\theta_j}{4N} \in \mathbb{R}$ for all $i \neq j \in \{0, 1, \cdots, n\}$, the free energy functional then is

$$\underbrace{F(q)}_{\text{free energy}} := \underbrace{\int_{\Delta_n} \psi(\mathbf{x}) q(\mathbf{x}) d\mathbf{x}}_{\text{potential energy}} + \underbrace{\int_{\Delta_n} q(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{x}}_{\text{negative entropy}} \tag{3.8}$$

for a density function q on Δ_n.

As we assume $\theta_i > 0$ for all i, the partition function

$$\begin{aligned} Z(\boldsymbol{\theta}) &:= \int_{\Delta_n} e^{-\psi(\mathbf{y})} d\mathbf{y} = \int_{\Delta_n} (y^1)^{\theta_1 - 1} (y^2)^{\theta_2 - 1} \cdots (y^n)^{\theta_n - 1} (1 - y^1 - \cdots - y^n)^{\theta_0 - 1} d\mathbf{y} \\ &= Beta(\boldsymbol{\theta}) \end{aligned} \tag{3.9}$$

is finite, and the minimizer of the free energy is the Gibbs density

$$q_\infty(\mathbf{x}) := \frac{e^{-\psi(\mathbf{x})}}{Z(\boldsymbol{\theta})}. \tag{3.10}$$

Below, we shall consider the evolution of the free energy functional along the flow of densities

$$F(u(\cdot, t)) := \int_{\Delta_n} \psi(\mathbf{x}) u(\mathbf{x}, t) d\mathbf{x} + \int_{\Delta_n} u(\mathbf{x}, t) \log u(\mathbf{x}, t) d\mathbf{x} \tag{3.11}$$

3.2. **Mutation and selection.** We return to the case of general mutation rates $\frac{\theta_{ij}}{4N} \in \mathbb{R}$ for $i \neq j \in \{0, 1, \cdots, n\}$. In addition, we now also include selection and assume that the genotype $A^i A^j$ has fitness $1 + \frac{s_{ij}}{2N}$. Then $\mathbf{X}_t$ satisfies (see, for instance, [10])

$$\begin{aligned} \mathbb{E}(\delta X_t^i | \mathbf{X}_t) &= b^i(\mathbf{X}_t)(\delta t) + o(\delta t); \\ \mathbb{E}(\delta X_t^i \delta X_t^j | \mathbf{X}_t) &= a^{ij}(\mathbf{X}_t)(\delta t) + o(\delta t), \quad \forall i, j = 1, \ldots, n; \\ \mathbb{E}((\delta \mathbf{X}_t)^{\boldsymbol{\alpha}} | \mathbf{X}_t) &= o(\delta t), \quad \text{for } |\boldsymbol{\alpha}| \geq 3, \end{aligned} \tag{3.12}$$

with the drift term

$$b^i(\mathbf{x}) = -\Big(\sum_{j=0}^n \frac{1}{2} \theta_{ij} \Big) x^i + \sum_{j=0}^n \frac{1}{2} \theta_{ji} x^j + s_i(\mathbf{x}) x^i - s(\mathbf{x}) x^i, \quad i = 1, \ldots, n; \tag{3.13}$$

with

$$s_i(\mathbf{x}) = \sum_{j=0}^n s_{ij} x^j \tag{3.14}$$

and

$$s(\mathbf{x}) = \sum_{i=0}^n s_i(\mathbf{x}) x^i; \tag{3.15}$$

and the diffusion term

$$a^{ij}(\mathbf{x}) = x^i(\delta_{ij} - x^j) \quad i, j = 1, \ldots, n.$$

We then have the following extension of Theorem 3.2.

Theorem 3.3. *In a diploid Wright–Fisher model of N individuals with $n+1$-alleles with mutation and selection, a necessary and sufficient condition for the existence of a unique stationary distribution is*

$$\theta_{ij} = \theta_j > 0 \quad \text{for all } i \neq j, \quad i, j = 0, \ldots, n \tag{3.16}$$

and

$$s_{ij} = s_{ji} \text{ for all } i, j. \tag{3.17}$$

The stationary distribution in this case is of the form

$$\mu_\infty^{m,s}(d\mathbf{x}) = f_\infty^{m,s}(\mathbf{x})d\mathbf{x} = \frac{e^{-\psi(\mathbf{x})}}{Z(\boldsymbol{\theta}, s)}d\mathbf{x} = \frac{\Pi_{i=0}^n (x^i)^{\theta_i - 1} e^{s(\mathbf{x})}}{Z(\boldsymbol{\theta}, s)}d\mathbf{x}, \tag{3.18}$$

with the partition function

$$Z(\boldsymbol{\theta}, s) = \int_{\Delta_n} \Pi_{i=0}^n (x^i)^{\theta_i - 1} e^{s(\mathbf{x})} d\mathbf{x}$$

While the condition on the uniformity of the mutation rates is somewhat restrictive, and in fact, biologically not entirely plausible (but standard in mathematical population genetics), the symmetry condition (3.17) is much more harmless. It simply that the allele combination A^iA^j has the same fitness as A^jA^i, i.e., that the fitness does not depend on the order of the alleles.

Proof. As in the proof of Theorem 3.2, ψ exists if and only if for all $i \neq k$

$$\partial_k\Big(f_i(\mathbf{x}) - f_0(\mathbf{x})\Big) = \partial_i\Big(f_k(\mathbf{x}) - f_0(\mathbf{x})\Big), \tag{3.19}$$

where

$$f_i(\mathbf{x}) = \frac{1 - 2b^i(\mathbf{x})}{x^i}. \tag{3.20}$$

Since we have already handled the mutation terms in (3.19) and shown that for them, (3.2) is necessary and sufficient, we only need to look at the contributions from selection. From (3.13), (3.14), this contribution is

$$\begin{aligned}
\tfrac{\partial}{\partial x^k}(s_i(x) - s(x) - s_0(x) - s(x)) &- \tfrac{\partial}{\partial x^i}(s_k(x) - s(x) - s_0(x) - s(x)) \\
&= \tfrac{\partial s_i(x)}{\partial x^k} - \tfrac{\partial s_0(x)}{\partial x^k} - \tfrac{\partial s_k(x)}{\partial x^i} + \tfrac{\partial s_0(x)}{\partial x^i} \\
&= s_{ik} - s_{0k} - s_{i0} + s_{00} - s_{ki} + s_{0i} + s_{k0} - s_{00}
\end{aligned}$$

which vanishes if and only if the symmetry condition (3.17) holds for all indices.

In the case of uniform mutation rates, then

$$b_i(\mathbf{x}) = \frac{\theta_i}{2} - \frac{|\boldsymbol{\theta}|}{2}x^i + s_i(\mathbf{x})x^i - s(\mathbf{x})x^i.$$

Therefore we can easily calculate the potential energy function as

$$\psi(\mathbf{x}) = \sum_{i=0}^n (1 - \theta_i)\log(x^i) - s(\mathbf{x}). \tag{3.21}$$

which follows from

$$\begin{aligned}\partial_i\psi(\mathbf{x}) &= \frac{1-2b_i(\mathbf{x})}{x^i} - \frac{1-2b_0}{x^0}\\ &= \left(\frac{1-\theta_i}{x^i} + |\boldsymbol{\theta}| - 2(s_i(\mathbf{x}) - s(\mathbf{x}))\right) - \left(\frac{1-\theta_0}{x^0} + |\boldsymbol{\theta}| - 2(s_0(\mathbf{x}) - s(\mathbf{x}))\right)\\ &= \frac{1-\theta_i}{x^i} - \frac{1-\theta_0}{x^0} - 2(s_i(\mathbf{x}) - s_0(\mathbf{x}))\end{aligned} \tag{3.22}$$

□

We now assume that the selection coefficients are of the form

$$s_{ij} = \frac{s_i + s_j}{2}. \tag{3.23}$$

This means that the fitness of a pair A^iA^j is the average of the fitness values of the individual alleles. In biological terms, this assumption is much more restrictive than the simple symmetry condition (3.17).

When (3.23) holds, (3.14), (3.15) become

$$s(x) = \sum_{j,k} \frac{s_j + s_k}{2} x^j x^k = \sum_j s_j x^j \tag{3.24}$$

since $\sum_k x^k = 1$.

Therefore, (3.21) becomes

$$\psi(\mathbf{x}) = \sum_{i=0}^{n}(1-\theta_i)\log(x^i) - \sum_{i=0}^{n} s_i x^i, \quad \text{where } x^0 = 1 - x^1 - \cdots - x^n.$$

In this case, the partition function for the free energy becomes

$$Z(\boldsymbol{\theta}, s) := \int_{\Delta_n} e^{-\psi(\mathbf{y})} d\mathbf{y} = \int_{\Delta_n} (y^1)^{\theta_1 - 1}(y^2)^{\theta_2 - 1}\cdots(y^n)^{\theta_n - 1}(1 - y^1 - \cdots - y^n)^{\theta_0 - 1} e^{\sum_{i=0}^{n} s_i y^i} d\mathbf{y}, \tag{3.25}$$

and Z is finite if and only if $\theta_i > 0$ for all $i = 0, \ldots, n$. In that case again, the minimizer of the free energy is the Gibbs density

$$q_\infty(\mathbf{x}) := \frac{e^{-\psi(\mathbf{x})}}{Z(\boldsymbol{\theta}, s)}. \tag{3.26}$$

4. Flow of free energies

Now we consider the evolution of the free energy along the flow of densities $\{u(\cdot, t)\}_{t \geq 0}$

$$F(u(\cdot, t)) := \int_{\Delta_n} \psi(\mathbf{x}) u(\mathbf{x}, t) d\mathbf{x} + \int_{\Delta_n} u(\mathbf{x}, t) \log u(\mathbf{x}, t) d\mathbf{x} \tag{4.1}$$

We know from the last section that in order to have a unique stationary reversible density we need to assume uniform positive mutation rates. So, in this section we shall alway assume that.

First, we recall an integration by parts formula.

Proposition 4.1.

$$\int_{\Delta_n} f(\mathbf{x})\nabla\cdot(A(\mathbf{x})Z(\mathbf{x}))d\mathbf{x} = -\int_{\Delta_n} A(\mathbf{x})\nabla f(\mathbf{x})\cdot Z(\mathbf{x}) \tag{4.2}$$

for all $f \in C^2(\overline{\Delta}_n)$ and Z is a vector field on $\overline{\Delta}_n$.

Proof. See [26] Proposition 2.4. □

We then prove that the free energy functional plays the role of the Lyapunov functional.

Lemma 4.2. *$F(u(\cdot,t))$ decreases along the flow of densities.*

Proof. Using the divergence form of the flow (3.5), we have

$$\frac{\partial}{\partial t}F(u(\cdot,t)) = \int_{\Delta_n}\psi(\mathbf{x})\frac{\partial}{\partial t}u(\mathbf{x},t)d\mathbf{x} + \int_{\Delta_n}\log u(\mathbf{x},t)\frac{\partial}{\partial t}u(\mathbf{x},t)d\mathbf{x} + \underbrace{\int_{\Delta_n}\frac{\partial}{\partial t}u(\mathbf{x},t)d\mathbf{x}}_{=0}$$

$$\begin{aligned}
&= \int_{\Delta_n}\psi(\mathbf{x})\nabla\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t))d\mathbf{x} + \psi(\mathbf{x})\nabla\cdot(A(\mathbf{x})u(\mathbf{x},t)\nabla\psi(\mathbf{x}))d\mathbf{x}\\
&\quad + \int_{\Delta_n}\log u(\mathbf{x},t)\nabla\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t))d\mathbf{x} + \log u(\mathbf{x},t)\nabla\cdot(A(\mathbf{x})u(\mathbf{x},t)\nabla\psi(\mathbf{x}))d\mathbf{x}\\
&= -\int_{\Delta_n}\nabla\psi(\mathbf{x})\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t))d\mathbf{x} - \nabla\psi(\mathbf{x})\cdot(A(\mathbf{x})u(\mathbf{x},t)\nabla\psi(\mathbf{x}))d\mathbf{x}\\
&\quad - \int_{\Delta_n}\nabla\log u(\mathbf{x},t)\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t))d\mathbf{x} - \nabla\log u(\mathbf{x},t)\cdot(A(\mathbf{x})u(\mathbf{x},t)\nabla\psi(\mathbf{x}))d\mathbf{x}\\
&\quad\text{(due to (4.2))}\\
&= -\int_{\Delta_n}\nabla\psi(\mathbf{x})\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t))d\mathbf{x} - \nabla\psi(\mathbf{x})\cdot(A(\mathbf{x})u(\mathbf{x},t)\nabla\psi(\mathbf{x}))d\mathbf{x}\\
&\quad - \int_{\Delta_n}\frac{\nabla u(\mathbf{x},t)\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t))}{u(\mathbf{x},t)}d\mathbf{x} - \nabla u(\mathbf{x},t)\cdot A(\mathbf{x})\nabla\psi(\mathbf{x})d\mathbf{x}\\
&= -\int_{\Delta_n} I(\mathbf{x},t)d\mathbf{x}
\end{aligned} \tag{4.3}$$

where

$$\begin{aligned}
I(\mathbf{x},t) &= u(\mathbf{x},t)\nabla\psi(\mathbf{x})\cdot(A(\mathbf{x})\nabla\psi(\mathbf{x})) + \frac{1}{u(\mathbf{x},t)}\nabla u(\mathbf{x},t)\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t))\\
&\quad + 2\nabla\psi(\mathbf{x})\cdot(A(\mathbf{x})\nabla u(\mathbf{x},t))\\
&= u < \nabla\psi,\nabla\psi >_{A(\mathbf{x})} + \frac{1}{u} < \nabla u,\nabla u >_{A(\mathbf{x})} + 2 < \nabla\psi,\nabla u >_{A(\mathbf{x})}\\
&\geq 0.
\end{aligned} \tag{4.4}$$

This completes the proof. □

Remark 4.3. We note that in our case $A(\mathbf{x})$ does not satisfy a uniform ellipticity condition as in [4]. In fact, when $\mathbf{x}$ goes to the boundary $\partial\Delta_n$, the Fisher information metric goes to infinity, and therefore $A(x)$ goes to 0.

We assume that there exists a unique stationary distribution $\mu_\infty(d\mathbf{x}) = u_\infty(\mathbf{x})d\mathbf{x}$. We focus on the rate of the convergence of u to u_∞. Putting

$$h := \frac{u}{u_\infty},$$

we shall investigate the rate of the convergence of h to 1.

The stationary density is the Gibbs density function

$$u_\infty(\mathbf{x}) = \frac{e^{-\psi(\mathbf{x})}}{Z},$$

which is an exponential family.

Thus

$$\log u_\infty + \psi = -\log Z.$$

Since Z is independent of $\mathbf{x}$, this implies

$$\partial_j(\log u + \psi) = \partial_j\Big(\log \frac{u}{u_\infty}\Big) + \partial_j(\log u_\infty + \psi) = \partial_j(\log h).$$

We now derive a partial differential equation for h from that of u

Lemma 4.4.

$$\partial_t h = \nabla\cdot(A(\mathbf{x})\nabla h) - \nabla\psi\cdot A(\mathbf{x})\nabla h = L^* h.$$

Proof. We have

$$\begin{aligned}
\partial_t h &= u_\infty^{-1}\partial_t u \\
&= u_\infty^{-1}\partial_i\Big(A^{ij}u\partial_j\big(\log u + \psi\big)\Big) \\
&= u_\infty^{-1}\partial_i\Big(A^{ij}u_\infty h\partial_j\big(\log h\big)\Big) \\
&= \partial_i\Big(A^{ij}h\partial_j\big(\log h\big)\Big) + u_\infty^{-1}\partial_i(u_\infty)\Big(A^{ij}h\partial_j\big(\log h\big)\Big) \\
&= \partial_i\Big(A^{ij}\partial_j h\Big) + \partial_i(\log u_\infty)\partial_i\Big(A^{ij}\partial_j h\Big) \\
&= \nabla\cdot(A(\mathbf{x})\nabla h) - \nabla\psi\cdot A(\mathbf{x})\nabla h
\end{aligned} \tag{4.5}$$

This completes the proof. □

Then, we can easily see that

$$\mu_\infty(d\mathbf{x}) = u_\infty(\mathbf{x})d\mathbf{x} = \frac{e^{-\psi(\mathbf{x})}}{Z}d\mathbf{x}$$

is reversible with respect to L^*.

Lemma 4.5.

$$\int_{\Delta_n} f L^* g d\mu_\infty = \int_{\Delta_n} g L^* f d\mu_\infty, \quad \forall f, g \in C^2(\Delta_n).$$

Proof.

(4.6)

$$\begin{aligned}\int_{\Delta_n} f L^* g d\mu_\infty &= \int_{\Delta_n} f\Big(\nabla\cdot(A(\mathbf{x})\nabla g)\Big)u_\infty(\mathbf{x})d\mathbf{x} - \int_{\Delta_n} f\Big(\nabla\psi\cdot A(\mathbf{x})\nabla g\Big)u_\infty(\mathbf{x})d\mathbf{x}\\ &= -\int_{\Delta_n} A(\mathbf{x})\nabla g\cdot\nabla\Big(f\frac{e^{-\psi(\mathbf{x})}}{Z}\Big)d\mathbf{x} - \int_{\Delta_n}\Big(\nabla\psi\cdot A(\mathbf{x})\nabla g\Big)f u_\infty(\mathbf{x})d\mathbf{x}\\ &\quad\text{(due to (4.2))}\\ &= -\int_{\Delta_n} A(\mathbf{x})\nabla g\cdot\Big(\nabla f - f\nabla\psi(\mathbf{x})\Big)\frac{e^{-\psi(\mathbf{x})}}{Z}d\mathbf{x} - \int_{\Delta_n}\Big(\nabla\psi\cdot A(\mathbf{x})\nabla g\Big)f u_\infty(\mathbf{x})d\mathbf{x}\\ &= -\int_{\Delta_n} A(\mathbf{x})\nabla g\cdot\nabla f\frac{e^{-\psi(\mathbf{x})}}{Z}d\mathbf{x}\\ &= -\int_{\Delta_n} A(\mathbf{x})\nabla g\cdot\nabla f d\mu_\infty(\mathbf{x}).\end{aligned}$$

which is symmetric between f and g. This yields the proof. □

We can now compute the decay rate of the free energy functional towards its asymptotic limit along the evolution of the probability density function u. For simplicity, we shall write $F(t)$ in place of $F(u(\cdot,t))$.

Theorem 4.6. *The difference of the current and the final free energy is equal to the relative entropy (Kullback-Leibler divergence) between the corresponding densities and also equal to the (negative) entropy of their ratio with respect to the stationary probability measure:*

$$F(t,\boldsymbol{\theta}) - F_\infty(\boldsymbol{\theta}) = D_{\mathrm{KL}}(u\|u_\infty) = S_{\mu_\infty}(h) \geq 0.$$

Proof. We have

$$\begin{aligned}F(t,\boldsymbol{\theta}) &= \int_{\Delta_n} u(\log u + \psi)d\mathbf{x}\\ &= \int_{\Delta_n} u(\log u_\infty + \psi)d\mathbf{x} + \int_{\Delta_n} u(\log u - \log u_\infty)d\mathbf{x}\\ &= \int_{\Delta_n} u(-\log Z)d\mathbf{x} + \int_{\Delta_n} u\log\frac{u}{u_\infty}d\mathbf{x} \qquad (4.7)\\ &= -\log Z + \int_{\Delta_n} u\log\frac{u}{u_\infty}d\mathbf{x}\\ &= -\log Z + \int_{\Delta_n} h\log h d\mu_\infty\end{aligned}$$

and

$$F_\infty(\boldsymbol{\theta}) = F(u_\infty) = \int_{\Delta_n} u_\infty(\log u_\infty + \psi) = -\log Z.$$

This implies the proof. □

Theorem 4.7. *The rate of change of the free energy functional is equal to the negative of the entropy production or the negative of the Fisher information:*

$$\frac{d}{dt}S_{\mu_\infty}(h) = \partial_t F(t,\boldsymbol{\theta}) = -J_{\mu_\infty}(h) := -\int_{\Delta_n} \frac{A(x)\nabla h\cdot\nabla h}{h}d\mu_\infty.$$

Proof. We have

$$\begin{aligned}
\partial_t F(t,\boldsymbol{\theta}) &= \int_{\Delta_n} \partial_t u(\log u+\psi)d\mathbf{x} + \int_{\Delta_n} u\partial_t(\log u+\psi)d\mathbf{x}\\
&= \int_{\Delta_n} \partial_i\Big(A^{ij}u\partial_j\big(\log u+\psi\big)\Big)(\log u+\psi)d\mathbf{x} + \int_{\Delta_n}\partial_t u d\mathbf{x}\\
&\quad (\text{ because } \partial_t\psi = 0)\\
&= -\int_{\Delta_n} \Big(A^{ij}u\partial_j\big(\log u+\psi\big)\Big)\partial_i(\log u+\psi)d\mathbf{x} + \partial_t\Big(\int_{\Delta_n} u d\mathbf{x}\Big) \qquad (4.8)\\
&\quad (\text{ due to } (4.2)\ )\\
&= -\int_{\Delta_n} A^{ij}u\partial_j(\log h)\partial_i(\log h)d\mathbf{x}\\
&= -\int_{\Delta_n} \frac{A^{ij}\partial_j h\partial_i h}{h}u_\infty d\mathbf{x}.
\end{aligned}$$

Since $F(u_\infty)$ is independent of t, this completes the proof. □

5. Curvature-dimension conditions

5.1. **General setting.** We start with some general notions, see [3] again.

We consider an operator $(L, D(L))$ defined on a measure space (Ω,μ) of the form

$$Lf = a^{ij}(x)\partial_i\partial_j f + b^i(x)\partial_i f, \forall f\in\mathcal{A} = L^2(\Omega,\mu)\cap D(L).$$

Definition 5.1. The carré du champ operator of L is defined by

$$\Gamma(f,g) = \frac{1}{2}\Big(L(fg) - fLg - gLf\Big),\quad \forall f,g\in\mathcal{A} \tag{5.1}$$

and the iterated carré du champ operator of L is defined by

$$\Gamma_2(f,g) = \frac{1}{2}\Big(L\Gamma(f,g) - \Gamma(f,Lg) - \Gamma(g,Lf)\Big),\quad \forall f,g\in\mathcal{A}. \tag{5.2}$$

We will also denote $\Gamma(f,f) = \Gamma(f)$ and $\Gamma_2(f,f) = \Gamma_2(f)$ for short.

Definition 5.2. We say that L satisfies the curvature-dimension condition $CD(\rho,n)$ for $\rho > 0$ and $n\in[1,\infty]$ if for all $f\in\mathcal{A}$

$$\Gamma_2(f) \geq \rho\Gamma(f) + \frac{1}{n}(Lf)^2,\quad \mu - a.e. \tag{5.3}$$

We recall some background results.

Proposition 5.3 (Bochner-Lichnerowicz formula)**.** *For a Riemannian manifold* (Ω, g)*, the Laplacian and the Ricci curvature are related via*

$$\frac{1}{2}\Delta_g\Big(|\nabla f|^2\Big) = \nabla f \cdot \nabla\Big(\Delta_g f\Big) + |\nabla\nabla f|^2 + Ric_g(\nabla f, \nabla f), \tag{5.4}$$

for all smooth functions $f : \Omega \to \mathbb{R}$*.*

Proof. See [20], for instance. □

Proposition 5.4 (Hessian formula)**.** *For a Riemannian manifold* (Ω, g)*, we have the Hessian formula*

$$\nabla\nabla f(\nabla g, \nabla h) = \frac{1}{2}\Big(\Gamma(g, \Gamma(f, h)) + \Gamma(h, \Gamma(f, g)) - \Gamma(f, \Gamma(g, h))\Big), \tag{5.5}$$

for all smooth functions $f, g, h : \Omega \to \mathbb{R}$*.*

Proof. See [3], for instance. □

Proposition 5.5. *Consider an* $n-$*dimensional Riemannian manifold* (Ω, g) *with Riemannian measure* μ_g*. Let* $m \geq n$*, then* $L = \Delta_g + Z$ *satisfies* $CD(\rho, m)$*, i.e.*

$$\Gamma_2(f) \geq \rho\Gamma(f) + \frac{(Lf)^2}{m}, \forall f \in \mathcal{A} \quad \mu_g - a.e$$

if and only if

$$Ric(L) := Ric_g - \nabla_S Z \geq \rho g + \frac{1}{m-n} Z \otimes Z,$$

where

$$(\nabla_S Z)_{ij} := \frac{1}{2}\Big(\partial_i Z^j + \partial_j Z^i\Big), \quad i, j = 1, \cdots, n,$$

is the symmetric covariant derivative of the vector field Z *in the metric* g*.* $Ric(L)$ *is often called the generalized Ricci tensor.*

Remark 5.6.
(1) The case $m = n$ can only occur when $Z = 0$;
(2) The case $m = \infty$, $L \in CD(\rho, \infty)$, i.e. $\Gamma_2(f) \geq \rho\Gamma(f)$, occurs if and only if $Ric(L) \geq \rho g$;
(3) If $Z = -\nabla W \cdot \nabla$ then $Ric(L) = Ric_g + \nabla\nabla W$. Therefore $L \in CD(\rho, \infty)$ if and only if $Ric_g + \nabla\nabla W \geq \rho g$ which is a general result of Bakry and Emery[2] in the Riemannian setting. Moreover by denoting $w_1^{m-n} = e^{-W}$ we have the more general criterion $L \in CD(\rho, m)$ if and only if $Ric_m(L) := Ric_g - \frac{m-n}{w_1}\nabla\nabla w_1 \geq \rho g$.

Proof. This follows from the Bochner-Lichnerowicz and Hessian formulas. □

We note that for the above operator L, we always have

$$\Gamma(f, g) = a^{ij}\partial_i f \partial_j g.$$

We now recall some known transport inequalities, which will be helpful for our entropy estimates.

Proposition 5.7 (Csiszár-Kullback-Pinsker Inequality)**.** *If* μ *and* ν *are two probability distributions, then*

$$\|\mu - \nu\|_{TV} \leq \sqrt{\frac{1}{2}D_{\mathrm{KL}}(\mu\|\nu)} \tag{5.6}$$

where

$$\|\mu-\nu\|_{TV}=\sup\{|\mu(A)-\nu(A)| : A \textit{ is an event to which probabilities are assigned.}\}$$

is the total variation distance (or statistical distance) between μ and ν.

Proof. The following proof is taken from [12] (see also [6] for a more general setting). We may assume $D_{\mathrm{KL}}(\mu\|\nu)<+\infty$. With $f=\frac{d\mu}{d\nu}$ and $u=f-1$ we have

$$\int u\,d\nu=\int d\mu-\int d\nu=0.$$

Therefore

$$D_{\mathrm{KL}}(\mu\|\nu)=\int_{\mathbf{X}} f\log f\,d\nu=\int_{\mathbf{X}}\Big((1+u)\log(1+u)-u\Big)\,d\nu.$$

The function $\varphi(t)=(1+t)\log(1+t)-t$, satisfies $\varphi'(t)=\log(1+t)$ and $\varphi''(t)=\frac{1}{1+t}$, $t>-1$. So, using a Taylor expansion,

$$\varphi(t)=\int_0^t (t-x)\varphi''(x)\,dx=t^2\int_0^1\frac{1-s}{1+st}\,ds,\quad t>-1.$$

So,

$$D_{\mathrm{KL}}(\mu\|\nu)=\int_{\mathbf{X}\times[0,1]}\frac{u^2(x)(1-s)}{1+su(x)}\,ds\,d\nu(x).$$

By the Cauchy-Schwarz inequality,

$$\begin{aligned}&\Big(\int_{\mathbf{X}\times[0,1]}|u|(x)(1-s)\,d\nu(x)ds\Big)^2\\ &\qquad\le\int_{\mathbf{X}\times[0,1]}\frac{u(x)^2(1-s)}{1+su(x)}\,d\nu(x)ds\cdot\int_{\mathbf{X}\times[0,1]}(1-s)(1+su(x))\,d\nu(x)ds\\ &\qquad=\frac{D_{\mathrm{KL}}(\mu\|\nu)}{2}.\end{aligned}$$

Since $\|\nu-\mu\|_{TV}=\frac{1}{2}\int|1-f|\,d\mu$, the left-hand side equals $\|\nu-\mu\|_{TV}^2$ and this completes the proof.

□

Proposition 5.8. *If μ and ν are two probability distributions with Radon-Nikodym derivatives f and g with respect to ρ, then*

$$\|f-g\|_{L^1(\rho)}\le\sqrt{2D_{\mathrm{KL}}(\mu\|\nu)}. \tag{5.7}$$

Proof. It follows from (5.6) and the equality

$$\|\nu-\mu\|_{TV}=\frac{1}{2}\|f-g\|_{L^1(\rho)}.$$

□

5.2. **Applications.** We now consider the Kolmogorov backward operator on $\Omega = \Delta_n$ with $\mathcal{A} = C^2(\Delta_n)$:

$$L^* h = A^{ij}(x)\partial_i \partial_j h + b^i(x)\partial_i h.$$

where

$$A^{ij} = \frac{1}{2} x^i(\delta_{ij} - x^j)$$

and

$$b^i = \frac{\theta_i}{2} - \frac{|\boldsymbol{\theta}|}{2}.$$

We have $g_{ij} = 2(\frac{\delta_{ij}}{x^i} + \frac{1}{x^0})$ as our Riemannian metric on Δ_n which is the inverse of $A^{ij}(x)$. We note that this metric is twice the metric in [25] p. 82 (also see in [17] Chapter 3), but because the Ricci curvature tensor R_{ij} does not change when we change the metric by multiplying by a constant λ (although the sectional curvature will change by λ), then from the relation $R_{ij} = \rho g_{ij}$ (which holds since we have a constant curvature metric), the Ricci curvature ρ becomes $\frac{n-1}{8}$.

With this Riemannian metric, we can write our Kolmogorov backward operator in the form

$$L^* = \Delta_g - \nabla W \cdot \nabla,$$

where e^{-W} is the density of the reversible measure μ with respect to the Riemannian measure $\mu_g(dx) = |\det(A(x))|^{-\frac{1}{2}} dx$. We know that the only reversible measure in this case is μ_∞. Therefore we can obtain $W(x), w_1(x)$ by

$$e^{-W(x)} = \frac{\Gamma(\theta_0)\ldots\Gamma(\theta_n)}{2^{\frac{n}{2}}\Gamma(|\theta|)} \prod_{i=0}^{n} (x^i)^{\theta_i - \frac{1}{2}} = w_1^{m-n}(x)$$

We have

$$\Gamma(w_1, f) = A^{ij}(x)\partial_i w_1 \partial_j f = \frac{w_1}{2(m-n)} Zf, \tag{5.8}$$

where

$$Zf := \sum_{i=1}^{n} (c_i - |c| x^i)\partial_i f$$

is a vector field on Δ_n with $c_i = \theta_i - \frac{1}{2}$, $|c| = \sum_{i=0}^{n} c_i = |\theta| - \frac{n+1}{2}$.

Therefore

(5.9)
$$\begin{aligned}
Ric_m(L)(\nabla f, \nabla f) &= Ric_g(\nabla f, \nabla f) - \frac{m-n}{w_1}\nabla\nabla w_1(\nabla f, \nabla f) \\
&= \frac{n-1}{8}(\nabla f, \nabla f) - \frac{1}{2}\Big(2\Gamma(f, \Gamma(w_1, f)) - \Gamma(w_1, \Gamma(f,f))\Big) \text{ by the Hessian formula (5.5)} \\
&= \frac{n-1}{8}(\nabla f, \nabla f) - \Big(\frac{1}{4(m-n)}(Zf)^2 + \frac{1}{2}A^{ij}(x)\partial_i f \partial_j (Zf) \\
&\quad - \frac{1}{2} Z(A^{ij}(x)\partial_i f \partial_j f)\Big) \text{ by (5.8)} \\
&= \frac{n-1+2|c|}{8}\Gamma(f) + \frac{1}{8}[c_i(\partial_i f - x^i \partial_i f)^2 + c_0(x^i\partial_i f)^2] - \frac{(Zf)^2}{4(m-n)}
\end{aligned}$$

Therefore, if $c_i \geq 0$ for all $i = 0, \dots, n$ i.e. $\theta_i \geq \frac{1}{2}$ for all $i = 0, \dots n$, then for $m \to \infty$ we have

$$Ric_\infty(L^*) \geq \frac{n-1+2|c|}{8} g = \rho_n g.$$

Thus, $L^* \in CD(\rho_n, \infty)$.

Remark 5.9. For $\theta_i = \frac{1}{2}$, i.e. $c_i = 0$, then $Zf = 0$ and $L^* = \Delta_g$ is the Laplacian; moreover

$$Ric_m(L) = Ric_g = \frac{n-1}{8} g$$

for all $m \geq n$. Therefore in this case, L^* satisfies $CD(\frac{n-1}{8}, n)$.

We can also directly calculate

$$\begin{aligned} \Gamma_2(f) &= |\nabla\nabla f|^2 + Ric(L^*)(\nabla f, \nabla f) \\ &= |\nabla\nabla f|^2 + Ric_g(\nabla f, \nabla f) + \nabla\nabla W(\nabla f, \nabla f) \end{aligned} \tag{5.10}$$

We now apply the Hessian formula (5.5) to calculate $\nabla\nabla W$. We have

$$W(x) = -\log \frac{2^{-\frac{n}{2}}}{Z} + \sum_{i=0}^{n} (\frac{1}{2} - \theta_i) \log x^i = -\log c + \sum_{i=0} d_i \log x^i$$

where

$$d_i = \frac{1}{2} - \theta_i, \quad |d| = \sum_{i=0}^{n} d_i = \frac{n+1}{2} - |\theta|.$$

Then

$$\partial_j W = \frac{d_j}{x^j} - \frac{d_0}{x^0}$$

and

$$A^{ij} \partial_j W = \frac{1}{2}(x^i \delta_{ij} - x^i x^j)(\frac{d_j}{x^j} - \frac{d_0}{x^0}) = \frac{1}{2}(d_i - |d| x^i).$$

This implies that

$$\Gamma(W, f) = A^{ij} \partial_i W \partial_j f = \frac{1}{2}(d_j - |d| x^j) \partial_j f.$$

Therefore

(5.11)

$$
\begin{aligned}
\nabla\nabla W(\nabla f,\nabla f) &= \Gamma(f,\Gamma(W,f)) - \frac{1}{2}\Gamma(W,\Gamma(f,f))\\
&= \frac{1}{2}A^{ij}\partial_i f\partial_j((d_k-|d|)\partial_k f) - \frac{1}{4}(d_k-|d|x^k)\partial_k\Big(A^{ij}\partial_i f\partial_j f\Big)\\
&= \frac{1}{2}A^{ij}\partial_i f\Big(-|d|\partial_j f\Big) - \frac{1}{4}(d_k-|d|x^k)\partial_k A^{ij}\partial_i f\partial_j f\\
&= -\frac{|d|}{2}|\nabla f|^2 - \frac{1}{8}(d_k-|d|x^k)(\delta_{ik}\delta_{ij}-\delta_{ik}x^j-\delta_{jk}x^i)\partial_i f\partial_j f\\
&= -\frac{|d|}{2}|\nabla f|^2 - \frac{1}{8}\Big(d_i(\partial_i f)^2 - |d|x^i(\partial_i f)^2 - 2d_i\partial_i f x^j\partial_j f + 2|d|(x^i)^2(\partial_i f)^2\Big)\\
&= -\frac{|d|}{2}|\nabla f|^2 - \frac{1}{8}\Bigg(\Big(d_i(\partial_i f)^2 - 2d_i\partial_i f x^j\partial_j f + |d|(x^i)^2(\partial_i f)^2\Big) - 2|d||\nabla f|^2\Bigg)\\
&= -\frac{|d|}{4}|\nabla f|^2 - \frac{1}{8}\Big(d_i(\partial_i f - Z_1 f)^2 + d_0(Z_1 f)^2\Big),\\
&= \frac{|c|}{4}|\nabla f|^2 + \frac{1}{8}\Big(c_i(\partial_i f - Z_1 f)^2 + c_0(Z_1 f)^2\Big),
\end{aligned}
$$

with the vector field

$$Z_1 f = x^i\partial_i f.$$

This implies that

$$\Gamma_2(f) = |\nabla\nabla f|^2 + Ric_g(\nabla f,\nabla f) + \frac{|c|}{4}|\nabla f|^2 + \frac{1}{8}\Big(c_i(\partial_i f - Z_1 f)^2 + c_0(Z_1 f)^2\Big).$$

If $c_i \geq 0$ for all $i = 0,\dots n$, i.e. $\theta_i \geq \frac{1}{2}$ for all $i = 0,\dots n$ then we obtain

$$\Gamma_2(f) \geq \frac{n-1+2|c|}{8}\Gamma(f) = \rho_n\Gamma(f). \tag{5.12}$$

It means that we have the curvature-dimension condition $CD(\rho_n,\infty)$, and that μ_∞ satisfies the $LSI(\rho_n,\infty)$.

Note that

$$\rho_n = \frac{n-1+2|c|}{8}$$

is not optimal, because we have used the rather coarse estimate

$$c_i(\partial_i f - Z_1 f)^2 + c_0(Z_1 f)^2 \geq 0.$$

Remark 5.10. Let us try to find the optimal value for the case of 2 alleles ($n = 1$) (see also [27]). In this case, the Ricci curvature $\frac{n-1}{8}$ vanishes. We have

$$W(x) = -\log\frac{\Gamma(\theta_1)\Gamma(\theta_0)}{\sqrt{2}\Gamma(\theta_1+\theta_0)} + (\frac{1}{2}-\theta_1)\log x + (\frac{1}{2}-\theta_0)\log(1-x).$$

With the Riemannian metric $g(x) = \frac{2}{x(1-x)}$ on $\Delta_1 = (0,1)$, we have $\Gamma(f) = |\nabla f|^2 = \frac{1}{2}x(1-x)(\partial_x f)^2$ and the Hessian of W

$$\nabla\nabla W(\nabla f, \nabla f) = \frac{c_1 + c_0}{4}|\nabla f|^2 + \frac{1}{8}\Big(c_1(1-x)^2 + c_0 x^2\Big)(\partial_x f)^2, \tag{5.13}$$

where $c_1 = \theta_1 - \frac{1}{2}$ and $c_0 = \theta_0 - \frac{1}{2}$.

When $\theta_1, \theta_0 \geq \frac{1}{2}$, i.e. $c_0, c_1 \geq 0$, by the Cauchy inequality the minimal eigenvalue of the Hessian of W is

$$\rho_1 = \Big(\frac{\sqrt{c_1} + \sqrt{c_0}}{2}\Big)^2.$$

Proposition 5.11. *If L is symmetric with respect to the stationary measure μ and satisfies the $CD(\rho, \infty)$ condition then μ satisfies $LSI(\rho, \infty)$.*

Proof. From the preceding calculations. □

These results will allow us to reach very precise conclusions. For instance, we have

Theorem 5.12. *For the Wright–Fisher model with $n+1$ alleles and positive uniform mutation rates satisfying $\theta_i > \frac{1}{2}$ for all $i = 0, \ldots, n$, the stationary distribution $\mathbf{f}_\infty d\mathbf{x}$ satisfies the $LSI(\rho_n, \infty)$ with*

$$\rho_n = \frac{n - 1 + |c|}{4} = \frac{n - 3 + 2|\boldsymbol{\theta}|}{8}.$$

Proof. Applying the results of (5.12) and (5.11). □

Corollary 5.13. *Under the above assumptions, the family of densities $\{u(\cdot, t)\}_{t \geq 0}$ is hypercontractive with respect to μ_∞, i.e., for all p_t satisfying*

$$p_t - 1 = e^{2\rho t}(p_0 - 1),$$

we have

$$\left(\int_\Omega \big|u(x,t)\big|^{p_t} d\mu_\infty(x)\right)^{\frac{1}{p_t}} \leq \left(\int_\Omega \big|u(x,0)\big|^{p_0} d\mu_\infty(x)\right)^{\frac{1}{p_0}}.$$

Corollary 5.14. *Under the above assumptions, the measure μ_∞ has the spectral gap $SG(\rho)$.*

Corollary 5.15. *Under the above assumptions, the rate of convergence of the relative entropy $D_{\mathrm{KL}}(u\|u_\infty)$ is*

$$D_{\mathrm{KL}}(u(t)\|u_\infty) \leq e^{-2\rho t} D_{\mathrm{KL}}(u(0)\|u_\infty).$$

Combining this with (5.6) and (5.7) implies that

1. *$u(t)dx$ exponentially converges to $u_\infty dx$ with respect to total variation distance;*
2. *$u(t)dx$ exponentially converges to $u_\infty dx$ with respect to L^1-norm.*

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