Convexity properties of products of random nonnegative matrices

(Ising models/free energy/heteropolymers/age-structured populations/Markovian environments)

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ABSTRACT Consider a sequence of $N \times N$ random nonnegative matrices in which each element depends on a vector u of parameters. The *n*th partial product is the random matrix formed by multiplying, from right to left, the first *n* of these random matrices in order. Under certain conditions, the elements of the *n*th partial product grow asymptotically exponentially as *n* increases, and the logarithms of the discrete long-run growth rates are convex functions of *u*. These conditions are met by some models in statistical mechanics and demography. Consequently, the Helmholtz free energy is concave and the population growth rate is convex in these models.

In statistical mechanics, a one-dimensional Ising model (1) of randomly composed heteropolymers, which has been proposed to describe DNA, takes the form of products of random matrices (2). We establish the concavity of the Helmholtz free energy, and hence thermodynamic stability, for generalizations of this model. The methods apply to higher-dimensional random Ising models as well (3).

In demography, models of age-structured populations with Markovian birth and death rates also take the form of products of random matrices (4–8). We establish the convexity of the natural measures of population growth rate in these models.

These results follow from observations about products of random matrices that follow readily from known theorems.

General results

Let $R = (-\infty, +\infty)$; $R^+ = [0, \infty)$; $R^{++} = (0, \infty)$; $Z = \{1, 2, ...\}$; $R^+_{N,N}$ = the set of $N \times N$ matrices with elements in R^+ , for N in Z; R_q = the set of q-tuples with elements in R, for q in Z.

in Z; R_q = the set of q-tuples with elements in R, for q in Z. Let U be an open convex set in R_q . We say $f:R_q \rightarrow R$ is convex if for all u and v in U, for all h in [0, 1], $f(hu + (1 - h)v) \leq hf(u) + (1 - h)f(v)$. A function f that takes only positive values is log convex if log f is convex. Let F be the class of all log convex functions, together with the function identically zero in U.

Let A be an arbitrary nonempty index set. We shall think of an element a of A as one possible state of a stochastic process at one point in discrete time. Let B be the set of all sequences

 $b = (a_1, a_2, \ldots, a_n, \ldots), a_n$ in A for all n in Z.

We shall think of each b as a sample path of a discrete-time stochastic process.

Let $X:A \times U \to R_{N,N}^+$, and let $X_{ij}(a,u)$ be the i,j element of the matrix X(a,u). Let $Y:Z \times B \times U \to R_{N,N}^+$ be defined, for n in Z, by

$$\Upsilon(n,b,u) = \chi(a_n, u)\chi(a_{n-1}, u)\cdots\chi(a_1, u),$$

in which ordinary matrix multiplication is intended on the right. The matrix Y(n,b,u) has i,j element $Y_{ij}(n,b,u)$.

Assume B has a family of measurable subsets on which a probability measure is defined. Expectations E_b over all sample paths b are to be computed with respect to this probability measure.

For any matrix m, we let $||m|| = \max_i \Sigma_j |m_{ij}|$. We take log $0 = -\infty$ and abbreviate $\lim_{n\to\infty} to \lim_n \mathbb{I}$.

THEOREM 1. For every a in A and every i, j = 1, ..., N, let $X_{ij}(a,.): U \rightarrow R^+$ be a function in the class F. Then for every p in R^{++} , whenever the indicated expectations and limits exist, F also contains the following R^+ -valued functions with domain U:

(i)
$$Y_{ii}^{p}(n,b,.)$$
 and $||Y(n,b,.)||^{p}$;

(ii) $E_b(Y_{ii}^p(n,b,.))$ and $E_b(||Y(n,b,.)||^p)$;

and the following functions are convex:

(iii)
$$\log \lambda_{p}(.) = \lim_{n \to \infty} n^{-1} E_{b}[\log(||Y(n,b,.)||^{p})]$$

and $\lim_{n \to \infty} n^{-1} E_{b}[\log Y_{i}^{p}(n,b,.)];$

(iv)
$$\log \mu_{\mathbf{p}}(.) = \lim_{n \to \infty} n^{-1} \log \mathbf{E}_{\mathbf{b}}[\|\mathbf{Y}(\mathbf{n},\mathbf{b},.)\|^{\mathbf{p}}]$$

and $\lim_{n \to \infty} n^{-1} \log \mathbf{E}_{\mathbf{b}}[\mathbf{Y}_{\mathbf{i}}^{\mathbf{p}}(\mathbf{n},\mathbf{b},.)].$

The proof requires these facts:

LEMMA [Artin (9), as stated by Marshall and Olkin (10)]. Let U be an open convex set in R_q and let (c, d) be an interval in R. Let $\phi: U \times (c, d) \rightarrow R^+$ satisfy

(i) $\phi(u,t)$ is Borel-measurable in t for each fixed u;

(ii) $\log \phi(u,t)$ is convex in u for each fixed t.

If ν is a measure on the Borel subsets of (c, d) such that $\phi(u, .)$ is ν -integrable for each u in U, then $\log \int_{c}^{d} \phi(u,t) d\nu(t)$ is convex on U.

LEMMA [Kingman (11)]. F is closed under addition, multiplication and raising to any positive power. If, for each n, f_n belongs to F, then so does $f = \lim \sup f_n$.

Proof of Theorem 1: Because matrix multiplication entails only addition and multiplication, Kingman's lemma implies immediately that F contains i and that, in iii, the functions to which E_b is applied are convex. Artin's lemma guarantees that the expectations in ii belong to F and that the functions in ivare convex. \Box

Over the range of values of p for which the quantities in *Theorem 1 iii* and *iv* exist, these quantities are also convex functions of p, for fixed u.

Theorems 2 and 3 below assure the existence of the limits in *iii* and *iv* under conditions that are satisfied in scientific applications.

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Define a set M of matrices in $R_{N,N}^{\perp}$ to be an ergodic set (12) if there is a G in Z and a constant ρ in (0,1) such that every product of G matrices, with or without repetitions, from M is strictly positive and if, for each matrix m in M, min⁺ $(m)/\max(m) > \rho$, in which min⁺(m) is the smallest nonzero element of m and max(m) is the largest element of m.

No matrix in an ergodic set can have a row or column that is entirely zero.

THEOREM 2 [Furstenberg and Kesten (ref. 2, p. 462)]. For each u in U, let {X(a,u); a in A} be an ergodic set. Let the probability measure on B be such that, for all u, (X(a_n,u), n in Z) is a stationary, metrically transitive stochastic process and $E_b(max[0, log X_{ij}(a_1,u)]) < \infty$ for i,j = 1, ..., N. Then for every p in R⁺⁺ there exists a finite positive constant $\lambda_p(u)$ such that, for all i,j = 1, ..., N, with probability one—i.e., for almost all sample paths b—

$$log \lambda_{p}(u) = lim_{n} n^{-1} log[Y_{ij}^{p}(n,b,u)]$$

= lim_{n} n^{-1} E_{b}(log[Y_{ij}^{p}(n,b,u)]).

In this statement of the theorem, the replacement of the original condition AI of Furstenberg and Kesten (2) by Hajnal's concept of ergodic set (12) goes part way toward making explicit some remarks of Kingman (ref. 13, p. 892). Furstenberg and Kesten (2) prove *Theorem 2* for p = 1.

When p = 1, we abbreviate $\mu_1(.)$ to $\mu(.)$ and $\lambda_1(.)$ to $\lambda(.)$.

COROLLARY 1. Under the combined assumptions of Theorems 1 and 2, $\log \lambda_p(.)$ is convex, for all p > 0.

David Ruelle (personal communication) pointed out that Corollary 6.23 of ref. 14 gives a variational formula for $\log \lambda$, from which also convexity follows.

THEOREM 3. Let $A_0 = \{1, \ldots, s\}$, and let $A = A_0^2 = \{(k,l); k, l \text{ in } A_0\}$. Let $P = (p_{kl})$ be a fixed $s \times s$ aperiodic irreducible stochastic matrix $(\sum_{i=1}^{s} p_{kl} = 1)$. For each u in U, let $X_u = \{x(k,l,u); (k,l) \text{ in } A\}$ be an ergodic set, which contains s^2 matrices in $R_{N,N}^+$. Let

$$\mathbf{P}[\mathbf{X}(\mathbf{a}_{n+1},\mathbf{u}) = \mathbf{x}(\mathbf{k},\mathbf{l},\mathbf{u}) \mid \mathbf{X}(\mathbf{a}_n,\mathbf{u}) = \mathbf{x}(\mathbf{g},\mathbf{h},\mathbf{u})] = \mathbf{p}_{\mathbf{k}\mathbf{l}}\delta_{\mathbf{h}\mathbf{k}}$$

for all g, h, k, and l in A₀, where $\delta_{hk} = 1$ if h = k, $\delta_{hk} = 0$ if $h \neq k$. Then there exists $\mu(u)$ in R⁺⁺ such that, for all i,j = 1, ..., N,

$$log \mu(\mathbf{u}) = lim_{n} n^{-1} log \mathbf{E}_{\mathbf{b}}[\mathbf{Y}_{ij}(\mathbf{n}, \mathbf{b}, \mathbf{u})]$$
$$= lim_{n} n^{-1} log \mathbf{E}_{\mathbf{b}}[\|\mathbf{Y}(\mathbf{n}, \mathbf{b}, \mathbf{u})\|].$$

Proof. The factors $X(a_i, u)$, a_i in A, $i = 1, \ldots, n$, are determined by successive overlapping *pairs* of states of the Markov chain with transition matrix P. If P specifies an aperiodic ergodic Markov chain, as we assume, then the "expanded" process on successive pairs of states is also an aperiodic ergodic Markov chain (ref. 15, pp. 140–141). Following the line of argument in *Corollary 1* of ref. 6 (p. 466), which concerns products of matrices indexed by successive *single* states of a Markov chain, there exists a primitive matrix m(u) that has a simple positive eigenvalue of maximum modulus (by the Perron-Frobenius theorem), and that eigenvalue is $\mu(u)$. \Box

COROLLARY 2. Under the combined assumptions of Theorems 1 and 3, log $\mu(u)$ and log $\lambda_p(u)$ are convex in u.

It suffices to note that the assumptions of *Theorem 3* imply those of *Theorem 2*.

Suppose the index set A contains only a single element and X_u contains only a single matrix x(u). The stochastic process degenerates to $Y(n,b,u) = [x(u)]^n$ for every n. In *Theorems 1*, 2, and 3, $\lambda(u) = \mu(u)$ are both equal to the spectral radius or Perron-Frobenius root of x(u). The convexity asserted in *Corollary 2* is then identical to that in the theorem of Kingman (11).

THEOREM 4. Let $M = \{x(k); k = 1, ..., s\}$ be a finite ergodic set. Let $(X(a_n), n \text{ in } Z)$ be a sequence of matrices from M, chosen independently and identically distributed, with

$$P[X(a_n) = x(k)] = \pi_k, k = 1, ..., s,$$

and $\Sigma_k \pi_k = 1$. With

$$b = (a_1, a_2, \dots, a_n, \dots),$$

$$Y(n,b) = X(a_n) \cdots X(a_1), and$$

$$\mu = lim_n n^{-1} log E_b[||Y(n,b)||]$$

$$= lim_n n^{-1} log E_b[Y_{ij}(n,b)],$$

we have that μ is a convex function of the N-vector with ith element equal to $\sum_{k=1}^{s} \pi_k x_{ii}(k)$. [The elements of this vector are precisely those of the main diagonal of the averaged matrix $x^* = \sum_k \pi_k x(k)$.]

Proof. μ is the spectral radius of x^* (ref. 6, p. 467). The spectral radius of any square nonnegative matrix is a convex function of the main diagonal of the matrix (16, 17). Combining these two results gives **Theorem 4**. \Box

I have verified the convexity asserted in Corollary 2 and Theorem 4 in numerical examples. The computation of $\log \lambda(.)$, which requires the solution of an integral equation followed by an integration, is outlined in ref. 7 and described in greater detail in refs. 5 and 6. The computation of $\mu(.)$, which requires finding the spectral radius of a nonnegative matrix, uses the power method. Both computer programs have been confirmed by using examples (8) in which λ and μ are known analytically.

Further examples show that neither λ nor μ is necessarily a convex function of $x_{ii}(k)$ (all else held constant) when $(X(a_n), n \text{ in } Z)$ is Markovian but not independently and identically distributed. However, the examples studied so far are compatible with the conjecture that the analog of *Theorem 4* holds for $\lambda = \lim_{n \to \infty} n^{-1} E_b[\log Y_{ij}(n,b)]$, as well as for μ , even though, in these examples, $\lambda < \mu$.

Ising chains in random magnetic fields

We now establish the concavity of the mean free energy per site as a function of parameters in a one-dimensional Ising model of a randomly composed heteropolymer. Concavity assures thermodynamic stability (ref. 18, pp. 72–75; ref. 19). Because products of random matrices have also been used to calculate the mean free energy per site in a two-dimensional Ising model with a Hamiltonian containing random coefficients (3), the approach and result presented here only for one-dimensional lattices can be extended readily to higher dimensions. Convexity properties of systems of spins on a lattice in which certain randomly chosen sites are vacant (20) do not appear to contain the results that follow.

For concreteness, consider a long polymer with two types of monomeric units, 1 and 2. For example, in double-stranded DNA, type 1 might represent an adenine-thymine base pair and type 2 a guanine-cytosine base pair (21, 22). Assume this polymer is in a very dilute solution, so that interactions between polymers can be neglected. Assume each molecule has free ends—i.e., ignore effects at the end of a molecule. In each polymer, index the units in order from right to left 1, 2, Let $\epsilon_n = +1$ if unit *n* is of type 1, $\epsilon_n = -1$ if unit *n* is of type 2. Thus if unit *n* is of type *i*, $\epsilon_n = (-1)^{i+1}$. As in ref. 21 (pp. 883–884), for *n* in Z, let $p_{ij} > 0$ be the conditional probability that monomer n + 1 is of type *j*, given that monomer *n* is of type *i*, in which i = 1, 2 and j = 1, 2.

Assume that each monomer, whether of type 1 or type 2, may be in one of two states: an unbonded state (a coil state in DNA) associated with a spin $\mu_n = +1$ or a bonded state (a helical state in DNA) associated with a spin $\mu_n = -1$. [This use of μ_n , which is conventional, for the spin variables should cause no confusion with the use of $\mu_p(.)$ for the limits in *Theorem 1 to*, because we will not use the latter notation in this section.]

We emphasize that $(\epsilon_n, n \in Z)$ is a Markovian stochastic process that specifies the chemical composition of a polymer, whereas $(\mu_n, n \in Z)$ is a sequence of spin variables that specifies the configuration of a polymer.

Suppose that the partition function Z_n of the first *n* monomers in the polymer contains no more than nearest neighbor interactions. (Z_n is distinct from the set Z of positive integers.) Assume that the coupling between the monomeric units at positions *m* and *m* + 1, *m* \in Z, is described by a real number $J_m = J(\mu_{m+1}, \epsilon_{m+1}, \mu_m, \epsilon_m)$. Suppose that the function J that maps the 16 possible arguments ($\mu_{m+1}, \epsilon_{m+1}, \mu_m, \epsilon_m$) = (± 1 , ± 1 , ± 1 , ± 1) into the real numbers does not depend directly on the position *m*—i.e., J is translation invariant. J may be written as a polynomial with coefficients independent of *m* in which the variables $\mu_{m+1}, \epsilon_{m+1}, \mu_m, \epsilon_m$ appear with exponent 0 or 1 and the terms are of degree at most 4. Then (for n > 1)

$$Z_n = \sum_{\{\mu(n)\}} \exp\left(\beta \sum_{m=1}^{n-1} J_m\right),$$

in which the outer sum is over the set $\{\mu(n)\}$ of all possible spin *n*-tuples $\mu(n) = (\mu_n, \ldots, \mu_1)$ and β^{-1} is the product of Boltzmann's constant and absolute temperature T.

We rewrite Z_n as a product of random matrices, which depend on the types of successive overlapping pairs of monomeric units, by conditioning on the spin of the *n*th monomer. For n > 1, express $\Sigma_{\{\mu(n)\}}$ as $\Sigma_{\{(1,\mu(n-1))\}} + \Sigma_{\{(-1,\mu(n-1))\}}$ and correspondingly Z_n as $u_n + v_n$. Then $Z_{n+1} = u_{n+1} + v_{n+1}$, in which

$$u_{n+1} = \sum_{\{(\mu_{n+1}=1,\mu_n=1,\mu(n-1))\}} \exp\left[\beta \sum_{m=1}^n J_m\right] \\ + \sum_{\{(\mu_{n+1}=1,\mu_n=-1,\mu(n-1))\}} \exp\left[\beta \sum_{m=1}^n J_m\right] \\ \exp[\beta J(1,\epsilon_{n+1},1,\epsilon_n)]u_n + \exp[\beta J(1,\epsilon_{n+1},-1,\epsilon_n)]v_n,$$

and similarly

=

$$v_{n+1} = \exp[\beta J(-1,\epsilon_{n+1},1,\epsilon_n)]u_n + \exp[\beta J(-1,\epsilon_{n+1},-1,\epsilon_n)]v_n.$$

Let $A = \{a_1, a_2\}$ be an index set with a_i corresponding to a monomeric unit of type *i*, and let (a_i, a_j) indicate that a unit of type *i* at some position *m* on the right is immediately followed at position m + 1 on the left by a unit of type *j*. Let

$$Y(n) = \begin{pmatrix} u_n \\ v_n \end{pmatrix},$$

$$\begin{aligned} x(a_i,a_j) &= \\ \begin{pmatrix} \exp[\beta J(1,(-1)^{j+1},1,(-1)^{i+1})] \exp[\beta J(1,(-1)^{j+1},-1,(-1)^{i+1})] \\ \exp[\beta J(-1,(-1)^{j+1},1,(-1)^{i+1})] \exp[\beta J(-1,(-1)^{j+1},-1,(-1)^{i+1})] \end{pmatrix} \end{aligned}$$

$$\mathbf{P}[X(n + 1) = x(a_i, a_j) | X(n) = x(a_g, a_h)] = p_{ij} \delta_{hi}, g, h, i, j = 1, 2$$

For any fixed finite values of the parameters β and $J(\pm 1, \pm 1, \pm 1, \pm 1, \pm 1)$, the elements of $x(a_i,a_j)$ are all positive, so $M = \{x(a_i,a_j); (a_i,a_j) \in A^2\}$ is an ergodic set. Then Y(n + 1) = X(n + 1)Y(n), $Z_n = Y_1(n) + Y_2(n) = u_n + v_n$, and the mean free energy f per monomer is, with probability 1, $f = -\beta^{-1} \lim_{n \to \infty} n^{-1} \log Z_n$. Thus, from *Corollary 1*, over an open convex region of the parameters $J(\pm 1, \pm 1, \pm 1, \pm 1)$, f is a concave function jointly of these parameters, when temperature T is fixed. From

Corollary 1 in conjunction with ref. 18, p. 77, when the other parameters are held fixed, f is a concave function of T over any fixed finite interval of positive values of T.

The model of Morgenstern *et al.* (1) is the special case in which successive monomeric units are independently and identically distributed, $p_{i2} = c$, i = 1,2, for c in (0,1), and (except for the *n*th monomeric unit, which has a negligible effect on f) J has the special form

$$J(\mu_{m+1}, \epsilon_{m+1}, \mu_m, \epsilon_m) = h_1 \mu_m + h_2 \mu_m \epsilon_m + h_3 \mu_m \mu_{m+1},$$

for some constants h_1 , h_2 , h_3 .

According to ref. 1, averaging the logarithm of the partition function $E[\log Z_n]$ is appropriate for "quenched random disorder," in which the local chemical composition of a polymer is not altered in time by thermal fluctuations in the solution. Computing $\log E[Z_n]$ corresponds to "fully annealed random disorder," in which the local chemical composition in a polymer is not fixed. Our *Corollary 2* shows that, under the assumptions of this section, $\lim_n n^{-1} \log E[Z_n]$ is a convex function of β and $J(\pm 1, \pm 1, \pm 1, \pm 1)$ jointly.

If this analysis were repeated for heteropolymers randomly composed from t > 2 types of monomeric units, the ergodic set M would contain t^2 transfer matrices instead of 4. If, instead of two possible values of spin, S possible values of spin were allowed, each transfer matrix would be of order $S \times S$. The restriction to nearest-neighbor interactions can be relaxed to interactions with finite range (ref. 23, pp. 134–135). The same conclusions hold for these extensions.

Age-structured populations with Markovian vital rates

Models that satisfy the assumptions of *Corollary 2* have been proposed to describe large, closed, unisexual age-structured populations in which the birth and death rates (or vital rates) at any time depend jointly and stochastically on the rates at an earlier time (6, 7).

Let us interpret Corollary 2 first for a population with vital rates, contained in a matrix x(u) in $R_{N,N}^+$, that are constant in time, but depend on a parameter u. Then $\log \mu(u) = \log \lambda(u)$ = r(u) is known as the Malthusian parameter or the intrinsic rate of natural increase of the population. All elements $x_{ij}(u)$ of the "Leslie" matrix x(u) are 0 except possibly for those $x_{1j}(u)$ in the first row, which specify the effective birth rate of individuals in the *j*th age group, and those $x_{j+1,j}(u)$ below the main diagonal, which specify the proportion of individuals in age group *j* at time n - 1 who survive to age group j + 1 at time *n*. At least $x_{1N}(u)$ and $x_{1K}(u)$, in which *K* is relatively prime to *N*, and all $x_{j+1,j}(u)$ on the subdiagonal are assumed positive to guarantee that x(u) is primitive.

We now show that the positive elements of x(u) are log convex functions of parameters, indicated generically by u, that have natural demographic interpretations. The probability l_{s+1}/l_s that an individual of exact age (i.e., in continuous time R^+) s will survive to exact age s + 1 is commonly expressed in terms of an underlying continuous-time force of mortality m(s)at exact age s as

$$l_{s+1}/l_s = \exp\left[-\int_s^{s+1} m(s')ds'\right],$$

which is a log-linear function of the force of mortality m(.). [The conventional actuarial notation $\mu(.)$ for this force of mortality would cause too much confusion here.] If the individuals in the *j*th age group are a mixture of individuals with exact ages *s* in the interval (j - 1, j], then $x_{j+1,j}(u)$ is the same mixture of survival probabilities l_{s+1}/l_s , and hence is also a log-linear function of the force of mortality u = m(.) at any set of exact ages. (Here we extend u from a q-tuple to a continuous function

over an interval of exact ages.) In practice, $x_{j+1,j}(u)$ is computed by assuming a mixture of survival probabilities that is invariant in time.

The effective birth rates $x_{1f}(u)$ in the first row of x(u) are a mixture of age-specific fertility rates f(s) at exact age s. The mixing distribution is assumed constant in time. The mixture depends on the survival, which is a log-linear function of mortality, of individuals in the interval (0,1]. A parameterization of age-specific fertility rates due to Coale and Trussell (ref. 24, p. 190) for a human female population is

$$f(s) = G(s)n(s)e^{wv(s)},$$

in which G(s) is the cumulative proportion ever married by exact age s, n(s) is "natural fertility," v(s) is a characteristic pattern of departure from natural fertility, and w is the extent of that departure. In this parameterization, G(.), n(.) and v(.)are given functions of exact age and f(.) is log convex in w. Thus $x_{1j}(u)$ is log convex in u = (w,m(.)). Other parameterizations of age-specific fertility, for example, as the derivative of a Gompertz distribution function, have also been found useful (25).

Having suggested that a log convex parameterization of x(u)arises naturally in this demographic model, we now interpret the conclusions of Corollary 2, continuing to assume for the moment that vital rates are constant in time. Suppose that $x_{ij}(u)$ $= b_{ij}(1 + k_{ij})^u, -1 < k_{ij} < \infty, u \ge 0$. We refer to the elements $x_{ij}(0) = b_{ij}$ as the baseline vital rates. In x(1), the baseline vital rate b_{ij} has been multiplied by a factor $1 + k_{ij}$. In x(2), those changed rates have again been multiplied by the same factor. An immediate consequence of the theorem of Kingman (11) is $r(2) - r(1) \ge r(1) - r(0)$. For example, if a 10% decrease in an age-specific birth rate lowered r in a hypothetical population from 0.03 to 0.02, then a further 10% decrease in the same birth rate, all else held constant, could not lower r beyond 0.01. Similarly, if a 20% improvement in the survival of children increased r in a hypothetical population from 0.01 to 0.02, then a further 20% improvement in the same survival proportions, all else held constant, would raise r to at least 0.03. These results appear to be previously unknown in the classical theory of stable populations.

In age-structured populations with Markovian vital rates, log, $\mu(u)$ and log $\lambda(u)$ are not, in general, equal, and there is no unique natural analog of the Malthusian parameter (26). The results just described for r(u) hold for each of log $\mu(u)$ and log $\lambda(u)$.

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