

AN INEQUALITY WITH APPLICATIONS TO STATISTICAL ESTIMATION FOR PROBABILISTIC FUNCTIONS OF MARKOV PROCESSES AND TO A MODEL FOR ECOLOGY

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1. Summary. The object of this note is to prove the theorem below and sketch two applications, one to statistical estimation for (probabilistic) functions of Markov processes [1] and one to Blakley's model for ecology [4].

2. Result.

THEOREM. Let $P(x) = P(\{x_{ij}\})$ be a polynomial with nonnegative coefficients homogeneous of degree d in its variables $\{x_{ij}\}$. Let $x = \{x_{ij}\}$ be any point of the domain D : $x_{ij} \geq 0$, $\sum_{j=1}^{q_i} x_{ij} = 1$, $i = 1, \dots, p$, $j = 1, \dots, q_i$. For $x = \{x_{ij}\} \in D$ let $\mathfrak{I}(x) = \mathfrak{I}\{x_{ij}\}$ denote the point of D whose i, j coordinate is

$$\mathfrak{I}(x)_{ij} = \left(x_{ij} \frac{\partial P}{\partial x_{ij}} \right) / \sum_{j=1}^{q_i} x_{ij} \frac{\partial P}{\partial x_{ij}} \Big|_{(x)}.$$

Then $P(\mathfrak{I}(x)) > P(x)$ unless $\mathfrak{I}(x) = x$.

Notation. μ will denote a doubly indexed array of nonnegative integers: $\mu = \{\mu_{ij}\}$, $j = 1, \dots, q_i$, $i = 1, \dots, p$. x^μ then denotes $\prod_{i=1}^p \prod_{j=1}^{q_i} x_{ij}^{\mu_{ij}}$. Similarly, c_μ is an abbreviation for $c_{\{\mu_{ij}\}}$. The polynomial $P(\{x_{ij}\})$ is then written $P(x) = \sum_\mu c_\mu x^\mu$.

In our notation:

$$(1) \quad \mathfrak{I}(x)_{ij} = \left(\sum_\mu c_\mu \mu_{ij} x^\mu \right) / \sum_{j=1}^{q_i} \sum_\mu c_\mu \mu_{ij} x^\mu.$$

We wish to prove

$$(2) \quad P(x) = \sum_\mu c_\mu x^\mu \leq \sum_\mu c_\mu \prod_{i=1}^p \prod_{j=1}^{q_i} \mathfrak{I}(x)_{ij}^{\mu_{ij}}.$$

PROOF.

$$P(x) = \sum_\mu \left\{ c_\mu \prod_{i=1}^p \prod_{j=1}^{q_i} \mathfrak{I}(x)_{ij}^{\mu_{ij}} \right\}^{1/d+1} \times \left\{ \frac{d^{d+1}}{c_\mu} x^\mu \prod_{i=1}^p \prod_{j=1}^{q_i} \left(\frac{1}{\mathfrak{I}(x)_{ij}} \right)^{\mu_{ij}/d+1} \right\}.$$

We apply Hölder's inequality [6, p. 21] to obtain

$$(3) \quad P(x) \leq \left\{ \sum_\mu c_\mu \prod_{i=1}^p \prod_{j=1}^{q_i} \mathfrak{I}(x)_{ij}^{\mu_{ij}} \right\}^{1/d+1} \times \left\{ \sum_\mu c_\mu x^\mu \prod_{i=1}^p \prod_{j=1}^{q_i} \left(\frac{x_{ij}}{\mathfrak{I}(x)_{ij}} \right)^{\mu_{ij}/d} \right\}^{d/d+1}.$$

(In the last braces we have used $(x^\mu)^{d+1/d} = x^\mu \prod_{i=1}^p \prod_{j=1}^{q_i} x_{ij}^{\mu_{ij}/d}$.) Since $\sum_{j=1}^{q_i} \mu_{ij}/d = 1$ by homogeneity of P , we can apply the inequality of geometric and arithmetic means [6, p. 16] to the double products of the second brace of (3) to conclude:

$$(4) \quad \sum_\mu c_\mu x^\mu \prod_{i=1}^p \prod_{j=1}^{q_i} \left(\frac{x_{ij}}{\mathfrak{I}(x)_{ij}} \right)^{\mu_{ij}/d} \leq \sum_\mu c_\mu x^\mu \sum_{i=1}^p \sum_{j=1}^{q_i} \frac{\mu_{ij}}{d} \frac{x_{ij}}{\mathfrak{I}(x)_{ij}}.$$

We now substitute the definition (1) of $\mathfrak{I}(x)_{ij}$ in the expression on the right of (4) and interchange the order of summation to obtain:

$$\begin{aligned} \sum_\mu c_\mu x^\mu \sum_{i=1}^p \sum_{j=1}^{q_i} \frac{\mu_{ij}}{d} \frac{x_{ij}}{\mathfrak{I}(x)_{ij}} &= \frac{1}{d} \sum_\mu c_\mu x^\mu \sum_{i=1}^p \sum_{j=1}^{q_i} \mu_{ij} \mathfrak{I}(x)_{ij} \\ &= \left(\sum_{j_0=1}^{q_i} \sum_{\mu'} c_{\mu'} \mu'_{ij_0} x^{\mu'} \right) / \left(\sum_{\mu'} c_{\mu'} \mu'_{ij} x^{\mu'} \right) \\ &= \frac{1}{d} \sum_{i=1}^p \sum_{j=1}^{q_i} x_{ij} \left[\left(\sum_\mu \mu_{ij} c_\mu x^\mu \right) / \left(\sum_{\mu'} \mu'_{ij} c_{\mu'} x^{\mu'} \right) \right] \\ &\quad \cdot \sum_{j_0=1}^{q_i} \sum_{\mu'} c_{\mu'} \mu'_{ij_0} x^{\mu'}. \end{aligned}$$

For each $\langle i, j \rangle$ the expression within the brackets is $= 1$ and by hypothesis for each i , $\sum_{j=1}^{q_i} x_{ij} = 1$. Hence the whole last expression of (5) reduces to $(1/d) \sum_{i=1}^p \sum_{j=1}^{q_i} \sum_{j_0=1}^{q_i} \sum_{\mu'} c_{\mu'} \mu'_{ij_0} x^{\mu'}$. But this is just $(1/d) \sum_{i_0=1}^p \sum_{j_0=1}^{q_{i_0}} \partial P / \partial x_{i_0 j_0}$ so by the Euler theorem for homogeneous functions it is equal to $\sum_\mu c_\mu x^\mu$.

Finally, if we use this upper bound $\sum_\mu c_\mu x^\mu$ for the expression within the second braces in (3), raise both sides of (3) to the $(d+1)$ st power, and divide both sides of the resulting inequality by $(\sum_\mu c_\mu x^\mu)^d$ we obtain the desired inequality (2).

That $P(\mathfrak{I}\{x_{ij}\}) > P\{x_{ij}\}$ if $\{x_{ij}\} \neq \{\mathfrak{I}(x)_{ij}\}$ follows from (4) and the strictness of the inequality of geometric and arithmetic means if all summands are not equal.

3. **Application 1.** The first application of this theorem is to statistical estimation for (probabilistically) lumped Markov chains. Let S be the finite state space of a Markov chain. Let f be a function from S to R . Let $y \in R^T$, T an integer, be an observation. In [1] the problem is considered of estimating the transition probabilities a_{ij} for $i, j \in S$, given y .

Let $X = (f^T)^{-1}(y)$. $X \subseteq S^T$. For $x \in X$, $i, j \in S$, let $v_{ij}(x)$ be the number of times the pattern $\cdot, \cdot, \cdot, i, j, \cdot, \cdot, \cdot$ occurs in x . The function $P(\{a_{ij}\}) = \sum_{x \in X} \prod_{i,j \in S} a_{ij}^{v_{ij}(x)}$ may be interpreted as the "probability of observing y given the transition probabilities $\{a_{ij}\}$." Note that P is a homogeneous polynomial of degree T with nonnegative (integer) coefficients in the variables a_{ij} .

An iterative procedure for estimating the transition probabilities $\{a_{ij}\}$ given y is suggested in [1]. If $\{a_{ij}\}$ is an *a priori* estimate, let $A'_{ij} = (\sum_{x \in X} v_{ij}(x) \prod_{k,l \in S} a_{kl}^{v_{kl}(x)}) / P(\{a_{ij}\})$. A'_{ij} may be interpreted as the "a posteriori expected value of the frequency of transition from state i to state j given y and the *a priori* probabilities $\{a_{ij}\}$." Thus $A'_{ij} / \sum_j A'_{ij}$ may be thought of as an "a posteriori estimate of the transition probabilities given y ." Since

$$A'_{ij} / \sum_j A'_{ij} = a_{ij} (\partial P / \partial a_{ij}) / \sum_{j \in S} (\partial P / \partial a_{ij})$$

by our theorem applied to the transformation $\mathcal{S}\{a_{ij}\} = \{A'_{ij} / \sum_j A'_{ij}\}$ we conclude that $P(\mathcal{S}\{a_{ij}\}) \geq P(\{a_{ij}\})$. In other words the *a posteriori* estimate of transition probabilities increases the likelihood of the given observation y .

Various results on the convergence of hill climbing iteration procedures [2], [3], [5] may be adduced to show that for almost all starts successive iterations will converge to a connected component of the local maximum set of P . If P has only finitely many local maxima then successive iterates converge to a point.

This is the usual case in the more general situation considered in [1] in which the observation y , at time t is obtained from the Markov state x_t at time t according to $P(y_t = k | x_t = j) = b_{jk}$ where b_{jk} is an $s \times r$ stochastic matrix which is also to be estimated. Here the identifiability problem does not arise since, according to a theorem of Ted Petrie [7], "in general" no other (a_{ij}) , (b_{jk}) yields the same y probabilities as a given (a_{ij}^0) , (b_{jk}^0) (save for the $s!$ relabellings of states).

The second application is to some results of Blakley and Dixon [2], [3], [4]. Let Γ be a symmetric p -linear form on R^n that has nonnegative coefficients with respect to the standard basis for R^n . Let $g(\eta) = \Gamma(\eta, \eta, \dots, \eta)$ where η is a vector in R^n . Since g is then just a p th degree homogeneous polynomial with nonnegative coeffi-

cients of the components of η we may apply the theorem of this note to it. In Blakley's model g is the adaptation (rate of growth) of a population. The transformation in Blakley's model $\sigma(\eta) = \eta_i (\partial g(\eta) / \partial \eta_i) / p g(\eta)$ is the same as the transformation $\mathcal{S}\{x_{ij}\}$ where $x_{ij} = \eta_j$, $i = 1, j = 1, \dots, n$.

In Blakley's model if η is the distribution of genotypes at time t , then $\sigma(\eta)$ is the distribution at time $t+1$. Thus it follows from the theorem in this note with $i=1$ that adaptation is nondecreasing with time when evolution of the genotypes at a single locus is considered. Our theorem with $i > 1$ yields the same conclusion under natural hypotheses for evolution of the genotypes at several loci. This nondecreasing of the adaptation with time is clearly a desirable feature of the model.

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