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: $x_{ij}\geqq 0$, $\sum_{j=1}^{q_i} x_{ij}=1$, $i=1,\cdots,p$, $j=1,\cdots,q_i$. For $x=\{x_{ij}\}\in D$ let $\mathfrak{I}(x)=\mathfrak{I}\{x_{ij}\}$ denote the point of D whose i, j coordinate is*

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

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

Notation. μ will denote a doubly indexed array of nonnegative integers: $\mu=\{\mu_{ij}\}$, $j=1,\cdots,q_i$, $i=1,\cdots,p$. 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:

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

We wish to prove

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

PROOF.

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

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

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

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

(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 $\sum_{i=1}^{p} \sum_{j=1}^{q_i} \mu_{ij}/d \equiv 1$ 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:

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

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:

$$\begin{aligned} &\sum_{\mu} c_\mu x^\mu \sum_{i=1}^{p} \sum_{j=1}^{q_i} \frac{\mu_{ij}}{d} \frac{x_{ij}}{\mathfrak{I}(x)_{ij}} \\ &\quad = \frac{1}{d} \sum_{\mu} c_\mu x^\mu \sum_{i=1}^{p} \sum_{j=1}^{q_i} \mu_{ij} x_{ij} \\ &\quad \cdot \left(\sum_{j_0=1}^{q_i} \sum_{\mu'} c_{\mu'} \mu'_{ij_0} x^{\mu'} \right) \Big/ \left(\sum_{\mu'} c_{\mu'} \mu'_{ij} x^{\mu'} \right) \\ &\quad = \frac{1}{d} \sum_{i=1}^{p} \sum_{j=1}^{q_i} x_{ij} \left[\left(\sum_{\mu} \mu_{ij} c_\mu x^\mu \right) \Big/ \left(\sum_{\mu'} \mu'_{ij} c_{\mu'} x^{\mu'} \right) \right] \\ &\quad \cdot \sum_{j_0=1}^{q_i} \sum_{\mu'} c_{\mu'} \mu'_{ij_0} x^{\mu'}. \end{aligned} \tag{5}$$

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 $(1/d) \sum_{i=1}^{p} \sum_{j_0=1}^{q_i} \sum_{\mu'} c_{\mu'} \mu'_{ij_0} x^{\mu'}$. But this is just $(1/d) \sum_{ij_0} x_{ij_0} \cdot (\partial P / \partial x_{ij_0})$ so by the Euler theorem for homogeneous functions it is equal to $\Sigma_\mu c_\mu x^\mu$.

Finally, if we use this upper bound $\Sigma_\mu c_\mu x^\mu$ 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 $(\Sigma_\mu c_\mu x^\mu)^d$ we obtain the desired inequality (2).

That $P(\mathfrak{I}\{x_{ij}\}) > P\{x_{ij}\}$ if $\{x_{ij}\} \neq \{x_{ij}\}$ 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 $\nu_{ij}(x)$ be the number of times the pattern $\cdot, \cdot, \cdot, i, j, \cdot, \cdot, \cdot$ occurs in x. The function $P(\{a_{ij}\})=\sum_{x\in X}\prod_{i,j\in S}a_{ij}^{\nu_{ij}(x)}$ 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 $A'_{ij}=(\sum_{x\in X}\nu_{ij}(x)\prod_{k,l\in S}a_{kl}^{\nu_{kl}(x)}/P(\{a_{ij}\})$. 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 $A'_{ij}/\Sigma_j A'_{ij}$ may be thought of as an "*a posteriori* estimate of the transition probabilities given y." Since

$$A'_{ij}/\Sigma_j A'_{ij} = a_{ij}(\partial P/\partial a_{ij})/\Sigma_j a_{ij}(\partial P/\partial a_{ij})$$

by our theorem applied to the transformation $\mathfrak{I}\{a_{ij}\}=\{A'_{ij}/\Sigma A'_{ij}\}$ we conclude that $P(\mathfrak{I}\{a_{ij}\})\geqq P(\{a_{ij}\})$. 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_t at time t is obtained from the Markov state x_t at time t according to $P(y_t=k\mid x_t=j)=b_{jk}$ 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^0_{ij}), (b^0_{jk}) (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 $g(\eta)=\Gamma(\eta, \eta, \cdots, \eta)$ where η is a vector in R^n. Since g is then just a pth degree homogeneous polynomial with nonnegative coefficients 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 $\sigma(\eta) = \eta_i(\partial g(\eta)/\partial \eta_i)/pq(\eta)$ is the same as the transformation $\mathfrak{I}\{x_{ij}\}$ where $x_{ij} = \eta_j$, $i = 1$, $j = 1, \cdots, n$.

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.

References

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