1 Problem

The score function $Q_n(X \mid Y)$, where X refers to one random variable and Y is some proposed parent set for that variable, is regular if

$$H_n(X \mid U) \le H_n(X \mid U \cup V) \quad \Rightarrow \quad Q_n(X \mid U) \ge Q_n(X \mid U \cup V),$$

where $H_n(\cdot | \cdot)$ refers to conditional empirical entropy and U and V are some sets of random variables.

Let X be a categorical random variable with r possible values. Let U denote a possible parent set with q different combinations of values for the variables and V a parent set with m different configurations. Assume that we have observed n samples of (X, U, V) and $H_n(X \mid U) \leq H_n(X \mid U \cup V)$ holds.

We want to show that

$$Q_n^{qnml}(X\mid U) \geq Q_n^{qnml}(X\mid U\cup V).$$

The assumption about entropy implies that the maximized likelihood terms of the qnml-score are equal. In order to prove the claim it suffices to study the penalty terms, and we want to show that

$$\begin{array}{rcl} -[reg(n,rq)-reg(n,q)] & \geq & -[reg(n,rqm)-reg(n,qm)] \\ reg(n,rq)-reg(n,q) & \leq & reg(n,rqm)-reg(n,qm) \\ & & \frac{C(n,rq)}{C(n,q)} & \leq \frac{C(n,rqm)}{C(n,qm)}, \end{array}$$

where C(n,k) is the stochastic complexity for multinomial random variable with k categories. Since, trivially, $q \leq qm$, we can prove the claim by showing that the function $k \mapsto C(n,rk)/C(n,k)$ is increasing for arbitrary $r \geq 2$ and $n \geq 1$.

2 Stochastic complexity

We can represent C(n,k) via recursion

$$C(n,k) = C(n,k-1) + C(n,k-2)n/(k-2)$$

or by using the following formula

$$C(n,k) = \sum_{l=0}^{n} \frac{n^{l} (k-1)^{\overline{l}}}{n^{l} l!}$$
$$= \sum_{l=0}^{n-1} \frac{(n-1)^{l} k^{\overline{l+1}}}{n^{l+1} l!}$$

where $x^{\underline{l}}$ and $x^{\overline{l}}$ denote falling and rising factorials, respectively.

3 Case n = 2

$$\frac{C(2,rk)}{C(2,k)} = \frac{1 + (rk-1) + (rk-1)rk/4}{1 + (k-1) + (k-1)k/4} = \frac{r^2k^2 + 3rk}{k^2 + 3k},$$

and since

$$\frac{d}{dk}\left(\frac{C(2,rk)}{C(2,k)}\right) = \frac{3r(r-1)k^2}{(k^2+3k)^2} = \frac{3r(r-1)}{(k+3)^2} > 0$$

for every $r \geq 2$ and $k \geq 1$, the claim holds.

4 Case n = 3

$$\frac{C(3,rk)}{C(3,k)} = \frac{r^3k^2 + 9r^2k + 17r}{k^2 + 9k + 17} \text{ and}$$

$$\frac{d}{dk} \left(\frac{C(3,rk)}{C(3,k)} \right) = \frac{(r-1)r(153 + 34(r+1)k + 9rk^2)}{(17 + 9k + k^2)^2} > 0$$

5 Case n=4

$$\frac{C(4,rk)}{C(4,k)} = \frac{142r + 95r^2k + 18r^3k^2 + r^4k^3}{142 + 95k + 18k^2 + k^3}$$

It seems that the denominator of the derivative contains "always" a polynomial of k with positive coefficients, and since the nominator is some polynomial squared, the resulting quotient is always positive for arbitrary r.

6 Case general

We first derive a representation for C(n, k) as a polynomial of k. We utilize the fact that the rising factorial can be represented as polynomial using unsigned Stirling numbers of the first kind

$$C(n,k) = \sum_{l=0}^{n-1} \frac{(n-1)^{l} k^{l+1}}{n^{l+1} l!}$$

$$= \sum_{l=0}^{n-1} b_{l} k^{l+1}$$

$$= \sum_{l=0}^{n-1} b_{l} \left(\sum_{j=1}^{l+1} |s(l+1,j)| k^{j} \right)$$

$$= \sum_{l=0}^{n-1} \left(\sum_{j=1}^{n} b_{l} |s(l+1,j)| k^{j} \right)$$

$$= \sum_{j=1}^{n} \left(\sum_{l=0}^{n-1} b_{l} |s(l+1,j)| k^{j} \right)$$

$$= \sum_{j=1}^{n} \left(\sum_{l=0}^{n-1} b_{l} |s(l+1,j)| k^{j} \right)$$

$$= \sum_{j=1}^{n} a_{j}k^{j},$$

where s(x,y) denotes the Stirling number of the first kind and

$$a_j = \left(\sum_{l=0}^{n-1} \frac{(n-1)^l}{n^{l+1}l!} |s(l+1,j)|\right),$$

 $a_j \ge 0$ for all j (also it seems that $\sum_{j=1}^n a_j = 1$). On the row 4, we used the property of Stirling numbers: s(i,j) = 0 for all j > i. Similarly,

$$C(n, rk) = \sum_{j=1}^{n} a_j r^j k^j$$

Derivatives are obtained easily from this form

$$\frac{d}{dk}C(n,k) = \sum_{j=1}^{n} ja_j k^{j-1}$$
$$= \sum_{j=0}^{n-1} (j+1)a_{j+1}k^j$$

and

$$\frac{d}{dk}C(n,rk) = \sum_{j=1}^{n} ja_j r^j k^{j-1}$$
$$= \sum_{j=0}^{n-1} (j+1)a_{j+1} r^{j+1} k^j.$$

Consider next the products found in the derivative of the quotient. We obtain

$$\left(\frac{d}{dk}C(n,rk)\right)C(n,k) = \left(\sum_{j=0}^{n-1}(j+1)a_{j+1}r^{j+1}k^{j}\right)\left(\sum_{l=1}^{n}a_{l}k^{l}\right)$$
$$= \sum_{i=1}^{2n-1}\left(\sum_{j+l=i}(j+1)a_{j+1}r^{j+1}a_{l}\right)k^{i}$$

and

$$\left(\frac{d}{dk}C(n,k)\right)C(n,rk) = \left(\sum_{j=0}^{n-1}(j+1)a_{j+1}k^{j}\right)\left(\sum_{l=1}^{n}a_{l}r^{l}k^{l}\right)$$
$$= \sum_{i=1}^{2n-1}\left(\sum_{j+l=i}(j+1)a_{j+1}a_{l}r^{l}\right)k^{i}.$$

Subtracting these two expression yields

$$\left(\frac{d}{dk}C(n,rk)\right)C(n,k) - \left(\frac{d}{dk}C(n,k)\right)C(n,rk)$$

$$= \sum_{i=1}^{2n-1} \left(\sum_{j+l=i} (j+1)a_{j+1}r^{j+1}a_l\right)k^i - \sum_{i=1}^{2n-1} \left(\sum_{j+l=i} (j+1)a_{j+1}a_lr^l\right)k^i$$

$$= \sum_{i=1}^{2n-1} \left(\sum_{j+l=i} (j+1)a_{j+1}a_l(r^{j+1}-r^l)\right)k^i$$

which is the polynomial in the denominator of the derivative of C(n, rk)/C(n, k). Next, we study the coefficient of k^i , if $i \leq n$

$$\sum_{j+l=i} (j+1)a_{j+1}a_l(r^{j+1}-r^l) = \sum_{l=1}^i (i-l+1)a_{i-l+1}a_l(r^{i-l+1}-r^l)$$

$$= \sum_{l=1}^i (i-l+1)c_l$$

$$= \sum_{k=1}^{\lfloor i/2 \rfloor} (i-k+1)c_k + (i-(i-k+1)+1)c_{i-k+1}$$

$$= \sum_{k=1}^{\lfloor i/2 \rfloor} (i-k+1)c_k + kc_{i-k+1}$$

$$= \sum_{k=1}^{\lfloor i/2 \rfloor} (i-k+1)c_k - kc_k$$

$$= \sum_{k=1}^{\lfloor i/2 \rfloor} (i-2k+1)c_k.$$

On the first row, we re-wrote sum using only one running index. On the second row we denoted $c_l = a_{i-l+1}a_l(r^{i-l+1} - r^l)$. On the third row, we re-arranged the sum so that we are summing over pairs of terms of the original sum: the first and the last term, the second and the second to last, and so on. This resulting sum has $\lfloor i/2 \rfloor$ terms. We have to use the floor-function since if i is odd, there exists an index l' in the original sum such that $r^{i-l'+1} - r^{l'} = 0$. On the fifth row, we make use of the identity $c_k = -c_{i-k+1}$ which is straightforward to verify. From the last row, we can observe that every term of the sum is positive since i-2k+1 and $r^{i-k+1}-r^k$ are both positive if $k \leq (i+1)/2$ which holds since k ranges from 1 to $\lfloor i/2 \rfloor$.

Let us now consider the situation where $n < i \le 2n - 1$. We start with the special case where i = 2n - 1. Then, we have only one term in the sum

$$\sum_{j+l=i} (j+1)a_{j+1}a_l(r^{j+1}-r^l) = \sum_{l=n}^n (2n-1-l+1)a_{2n-1-l+1}a_l(r^{2n-1-l+1}-r^l)$$
$$= na_na_n(r^n-r^n)$$
$$= 0.$$

Now, let n < i < 2n-1, we follow a similar procedure as before to manipulate the sum

$$\begin{split} \sum_{j+l=i} (j+1)a_{j+1}a_l(r^{j+1}-r^l) &= \sum_{l=i-n+1}^n (i-l+1)a_{i-l+1}a_l(r^{i-l+1}-r^l) \\ &= \sum_{l=i-n+1}^n (i-l+1)c_l \\ &= \sum_{k=1}^{2n-i} (n-k+1)c_{i-n+k} \\ &= \sum_{k=1}^{\lfloor n-i/2\rfloor} (n-k+1)c_{i-n+k} \\ &+ (n-(2n-i-k+1)+1)c_{i-n+(2n-i-k+1)} \\ &= \sum_{k=1}^{\lfloor n-i/2\rfloor} (n-k+1)c_{i-n+k} + (i-n+k)c_{n-k+1} \\ &= \sum_{k=1}^{\lfloor n-i/2\rfloor} (n-k+1)c_{i-n+k} - (i-n+k)c_{i-n+k} \\ &= \sum_{k=1}^{\lfloor n-i/2\rfloor} (n-k+1-(i-n+k))c_{i-n+k} \\ &= \sum_{k=1}^{\lfloor n-i/2\rfloor} (2n-i-2k+1)c_{i-n+k}. \end{split}$$

It is now easy to verify that (2n - i - 2k + 1) and c_{i-n+k} are positive if $k \leq n - (i-1)/2$ which holds since k ranges from 1 to $\lfloor n - i/2 \rfloor$. The floor function is again used when we sum over pairs of terms since if i is odd there is zero-term. Since all the coefficients are non-negative and the $k \geq 2$, the derivative is positive. This implies that the original function is increasing.

7 Terms a_j sum to one

$$\sum_{j=1}^{n} a_{j} = \sum_{j=1}^{n} \left(\sum_{l=0}^{n-1} \frac{(n-1)^{l}}{n^{l+1}l!} |s(l+1,j)| \right)$$

$$= \sum_{l=0}^{n-1} \frac{(n-1)^{l}}{n^{l+1}l!} \left(\sum_{j=1}^{n} |s(l+1,j)| \right)$$

$$= \sum_{l=0}^{n-1} \frac{(n-1)^{l}}{n^{l+1}l!} \left(\sum_{j=0}^{l-1} |s(l+1,j)| \right)$$

$$= \sum_{l=0}^{n-1} \frac{(n-1)^{l}}{n^{l+1}l!} (l+1)!$$

$$= \sum_{l=0}^{n-1} \frac{(n-1)^{l}}{n^{l+1}} (l+1)$$