The Dimension of an Evolutionary Algorithm Transition Matrix

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Suppose that u and v are vectors that represent possible populations in an evolutionary algorithm. u and v each have n elements, where n is the cardinality of the search space, i.e., the total number of possible unique individuals. N is the population size, so that the sum of the elements of u is equal to N, and the sum of the elements of v is also equal to N.

The Markov transition matrix Q for an evolutionary algorithm gives the probability that the algorithm will transition from one population to another population after one generation. Q is therefore a $T \times T$ matrix, where T is the total number of possible population distributions. That is, T is the number of possible $n \times 1$ integer vectors whose elements sum to N and each of whose elements in in $[0, N]$. This number can be calculated several different ways. In [1] it is shown that T can be calculated with the choose function.

$$T = \begin{pmatrix} n+N-1 \\ N \end{pmatrix} \tag{1}$$

We can also use the multinomial theorem [2] to find T. The multinomial theorem can be stated in several ways, including the following. Given K classes of objects, the number of different ways that N objects can be selected (independent of order) while choosing from each class no more than M times is the coefficient q_N in the polynomial

$$\begin{aligned} q(x) &= (1 + x + x^2 + \cdots + x^M)^K \\ &= 1 + q_1 x + q_2 x^2 + \cdots + x^{MK} \end{aligned} \tag{2}$$

Recall that the population vector v is an n-element vector such that each element is an integer between 0 and N (inclusive), and the sum of its elements is N. T is the number of unique population vectors v. So T is the number of ways that N objects can be selected (independent of order) from n classes of objects while choosing from each class no more than N times. Applying the multinomial theorem to this problem gives

$$\begin{aligned} T &= q_N \\ q(x) &= (1 + x + x^2 + \cdots + x^N)^n \\ &= 1 + q_1 x + q_2 x^2 + \cdots + x^{Nn} \end{aligned} \tag{3}$$

A different form of the multinomial theorem can also be used to find T. The multinomial theorem can be stated as

$$\begin{aligned} (x_1 + x_2 + \cdots + x_N)^n &= \sum_{S(k)} \frac{n!}{\prod_{j=1}^{N} k_j!} \prod_{j=1}^{N} x_j^{k_j} \\ &= \sum_{S(k)} \prod_{i=1}^{N} \left(\begin{array}{c} \sum_{j=1}^{i} k_j \\ k_i \end{array} \right) \prod_{j=1}^{N} x_j^{k_j} \\ S(k) &= \left\{ k \in \mathbf{R}^N : k_j \in \{0, 1, \cdots, N\}, \sum_{j=1}^{N} k_j = n \right\} \end{aligned} \tag{4}$$

Now consider the polynomial $(x^0 + x^1 + x^2 + \cdots + x^N)^n$. From the multinomial theorem (4) we see that the coefficient of $[(x^0)^{k_0}(x^1)^{k_1}(x^2)^{k_2} \cdots (x^N)^{k_N}]$ is given by

$$\prod_{i=0}^{N} \left(\begin{array}{c} \sum_{j=0}^{i} k_j \\ k_i \end{array} \right) \tag{5}$$

If we sum up these terms for all k_j such that

$$\sum_{j=0}^{N} j k_j = N \tag{6}$$

then we obtain the coefficient of x^N. But (3) shows that T is equal to the coefficient of x^N. Therefore

$$\begin{aligned} T &= \sum_{S'(k)} \prod_{i=0}^{N} \left(\begin{array}{c} \sum_{j=0}^{i} k_j \\ k_i \end{array} \right) \\ S'(k) &= \{ k \in \mathbf{R}^{N+1} : k_j \in \{0, 1, \cdots, N\}, \sum_{j=0}^{N} k_j = n, \sum_{j=0}^{N} j k_j = N \} \end{aligned} \tag{7}$$

Equations (1), (3), and (7) give three different expressions for the dimension of the Markov transition matrix Q.

Example

Suppose that our population consists of two-bit individuals ($n = 4$) and a population size $N = 4$. Equation (1) gives

$$T = \left(\begin{array}{c} 7 \\ 4 \end{array} \right) = 35 \tag{8}$$

Equation (3) gives

$$\begin{aligned} q(x) &= (1 + x + x^2 + x^3 + x^4)^4 \\ &= 1 + \cdots + 35x^4 + \cdots + x^{16} \\ T &= q_4 = 35 \end{aligned} \tag{9}$$

Equation (7) gives

$$\begin{aligned} T &= \sum_{S'(k)} \prod_{i=0}^{4} \left(\begin{array}{c} \sum_{j=0}^{i} k_j \\ k_i \end{array} \right) \\ S'(k) &= \{k \in \mathbf{R}^5 : k_j \in \{0, 1, \cdots, 4\}, \sum_{j=0}^{4} k_j = 4, \sum_{j=0}^{4} j k_j = 4\} \\ &= \Big\{ \left(\begin{array}{ccccc} 3 & 0 & 0 & 0 & 1 \end{array} \right), \left(\begin{array}{ccccc} 2 & 1 & 0 & 1 & 0 \end{array} \right), \left(\begin{array}{ccccc} 2 & 0 & 2 & 0 & 0 \end{array} \right), \\ & \quad \left(\begin{array}{ccccc} 1 & 2 & 1 & 0 & 0 \end{array} \right), \left(\begin{array}{ccccc} 0 & 4 & 0 & 0 & 0 \end{array} \right) \Big\} \\ T &= 4 + 12 + 6 + 12 + 1 = 35 \end{aligned} \tag{10}$$

References

[1] A. Nix and M. Vose, Modeling genetic algorithms with Markov chains, Annals of Mathematics and Artificial Intelligence (5) pp. 79-88, 1992.

[2] C. Chuan-Chong and K. Khee-Meng, Principles and Techniques in Combinatorics, World Scientific, 1992.