LINEAR RECURRENCE RELATIONS WITH BINOMIAL COEFFICIENTS

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A linear recurrence relation of the n^{th} order is defined as

$$T_{i+n} = \sum_{j=1}^{n} a_j T_{i+n-j}, \qquad i = 0, 1, 2, \ldots, \tag{1}$$

where $a_1, a_2, \ldots, a_n$ are given coefficients. When all the coefficients are set equal to 1, the relation generates t-Fibonacci sequences [1], the Fibonacci sequence for $n = 2$, the Tribonacci sequence for $n = 3$ [2], and so on.

Another case arises when the coefficients in relation (1) are set equal to binomial coefficients, i.e.,

$$T_{i+n} = \sum_{j=1}^{n} \binom{n-1}{j-1} T_{i+n-j}. \tag{2}$$

For $n = 2$, relation (2) is reduced to the Fibonacci sequence and the recurring sequences generated by the recurrence relations with binomial coefficients (2) can be considered as another generalization of the Fibonacci sequence. These "binomial" sequences interest the author because of their relation to the dynamic development of self-replicating biochemical systems [3].

Consider self-replication of the type shown in Figure 1, i.e.,

$$A_1 \xrightarrow{k_1} A_2 + A_1 \tag{R1}$$

$$A_j \xrightarrow{k_j} A_{j+1}, \qquad j = 2, \ldots, n-1, \tag{Rj}$$

$$A_n \xrightarrow{k_n} A_1 \tag{Rn}$$

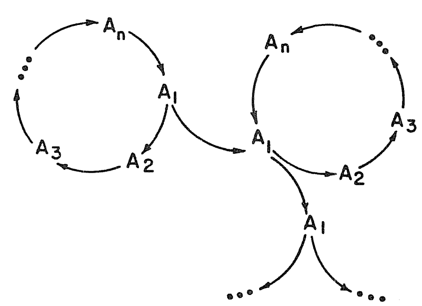

Figure 1. A Schematic Diagram of a Self-Replicating Process

Species A_1 forms species A_2 while reproducing itself in reaction (R1). Species A_2 undergoes $n-1$ transformations by reactions (R2)-(Rn) producing in the last step of this sequence the initial species A_1. Assume the first-order mass-action law for each of the reactions, that is, the rate of the j^{th} reaction is proportional to the concentration of species A_j, and also assume that the rate coefficients are identical, i.e., $k_j = k$ for $j = 1, 2, \ldots, n$, the differential equations which describe the kinetics of the system take the form

$$\frac{d[A_1]}{dt} = k[A_n], \qquad \frac{d[A_j]}{dt} = k[A_{j-1}] - k[A_j], \qquad j = 2, \ldots, n,$$

with initial conditions

$$[A_1]_{t=0} = C_0,$$
$$[A_j]_{t=0} = 0, \qquad j = 2, 3, \ldots, n,$$

where:

$[A_j]$ is the concentration of species A_j;

C_0 is the initial concentration of species A_1;

t is time.

Dividing both sides of each differential equation by kC_0 and introducing dimensionless variables

$$a_j = [A]_j/C_0 \qquad \text{for } j = 1, 2, \ldots, n$$

and $\quad \tau = kt,$

these equations can be rewritten as

$$\frac{da_1}{d\tau} = a_n, \quad \frac{da_j}{d\tau} = a_{j-1} - a_j, \qquad j = 2, \ldots, n,$$

with initial conditions

$$a_j \Big|_{\tau=0} = \delta_{1j}.$$

The characteristic equation for this system of differential equations is

$$r(r+1)^{n-1} - 1 = 0. \tag{3}$$

Thus, the roots of (3) determine the kinetics of the reaction sequence.

Returning to the "binomial" sequence (2), the auxiliary polynomial for this sequence is

$$x^n - \sum_{j=1}^{n} \binom{n-1}{j-1} x^{n-j} = 0 \quad \text{or} \quad x^n - (x+1)^{n-1} = 0. \tag{4}$$

Defining $r = 1/x$, (4) becomes (3). Analysis of the "binomial" sequences and their relations can provide information necessary for understanding self-replication of the type considered here. It would be of interest to determine all possible relationships between the roots of equation (4) and their dependence on the order n.

For example, defining $z = r + 1$, equation (3) becomes

$$z^n - z^{n-1} - 1 = 0. \tag{5}$$

Equation (5) and its solution are discussed in a number of articles [4]-[7]. From the results of Ferguson [6] and Hoggatt & Alladi [7], the following conclusions can be made for roots of equation (3):

Property 1: For all n, there exists only one positive real root r_1—the dominant root of (3)—such that

$$r_1 = 1/\phi_n \tag{6}$$

where

$$\phi_n = \lim_{i \to \infty} \frac{T_{i+1}}{T_i} \tag{7}$$

is the limiting ration of the "binomial" sequence of the n^{th} order.

Proof: It was proven in [6] and [7] that (5) has a single positive root with largest absolute value, λ_1. That is, λ_1 is the dominant root of (5). Since $r = z - 1$, $r_1 = \lambda_1 - 1$ is the dominant root of (3). Furthermore, since $x = 1/(z - 1)$, (4) has only one positive real root, $x_1 = 1/(\lambda_1 - 1)$. Root x_1 has the largest absolute value: It was proven in [6] that $\lambda_1 - 1 \leqslant |z - 1|$; therefore

$$\frac{1}{\lambda_1 - 1} \geqslant \frac{1}{|z - 1|} \qquad \text{or} \qquad x_1 \geqslant |x|.$$

Thus, there exists a single root of largest absolute value for (4); this satisfies the condition of the lemma in [7], proving the existence of limit (7) and that $x_1 = \phi_n$. Equation (6) follows from $x_1 = \phi_n$ and $r_1 = 1/x_1$.

Property 2: For n even, there is also one negative real root.

Proof: This follows from applying Descartes' Rule of Signs to equation (5) and using the relationship $r = z - 1$.

Property 3: $\lim\limits_{n \to \infty} r_1 = \lim\limits_{n \to \infty}(1/\phi_n) = 0$.

Proof: This follows from $r_1 = \lambda_1 - 1$ and the result of Theorem B in [6] that

$$\lim_{n \to \infty} \lambda_1 = 1.$$

Property 4: All the roots are distinct and lie in the intersection of the two annuli

$$\lambda_0 \leqslant |r_j + 1| \leqslant r_1 + 1 \quad \text{and} \quad r_1 \leqslant |r_j| \leqslant 1 + \lambda_0,$$

where r_j, $j = 2, 3, \ldots, n$, are the (complex) roots of equation (3) and λ_0 is the largest real solution of $u^n + u^{n-1} - 1 = 0$ $(0 < \lambda_0 < 1 < r_1 + 1 < 2)$.

Proof: These results follow from Theorem A in [6] and $r = z - 1$.

Species concentrations a_j are determined by linear combinations of n exponential terms $e^{r_\ell \tau}$, where r_ℓ $(\ell = 1, 2, \ldots, n)$ are the roots of (3). Based on properties (1)-(4) above, the dynamic behavior of reaction system (R1)-(Rn) is dominated by the term $e^{r_1 \tau}$ $(= e^{\tau/\phi_n})$. At $n \geqslant 14$ there are complex roots r_ℓ with positive real parts (e.g., $0.00617 \pm 0.38302i$), thus indicating the appearance of nondecaying, oscillatory components in the concentration profiles. The exponential term for a complex root takes the form $e^{\alpha\tau}e^{\beta\tau i}$, where $r = \alpha + \beta i$. The term $e^{\beta\tau i}$ indicates oscillatory behavior of species concentrations in time. If α is negative, oscillations are decaying with increase in τ. For $\alpha > 0$, the oscillatory behavior is nondecaying. More detailed general analysis of the reaction kinetics depends on whether the roots of (3) and their dependence on n can be isolated further. Thus, it would be of interest to determine the frequencies and amplitudes of oscillatory components in concentration profiles.

The following recurrence expression,

$$\frac{\log \phi_n}{\log \phi_{n-1}} \approx \frac{\log n}{\log(n - 1)}, \tag{8}$$

seems to be an approximate relationship between the limiting ratios (or the dominant roots) of different orders (see Figure 2). Since the dominant root of (3) is specified by ϕ_n, namely $r_1 = 1/\phi_n$, and the dominant root determines the main dynamic behavior of the reaction system, relationship (8) can be used to approximate such behavior. A question is: Can relationship (8) be justified and can it be improved?

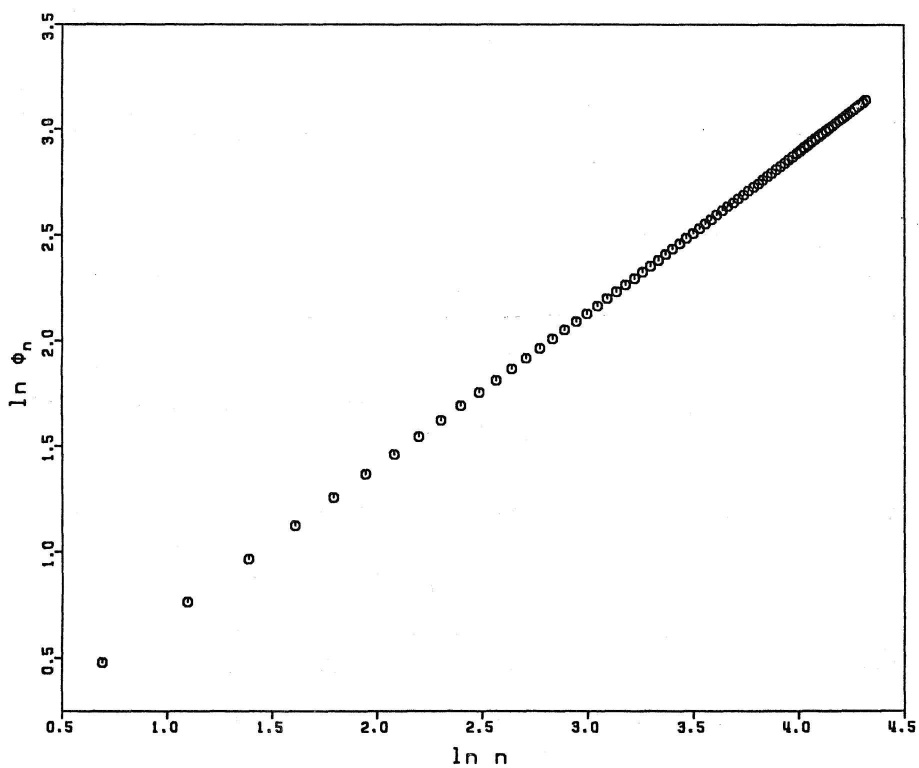

Figure 2. Logarithmic Dependence of the Limiting Ratio of the "Binomial" Sequence on the Order of the Sequence

The following proof that $\log \phi_n/\log n$ is bounded was suggested by the reviewer.

Conjecture: $\lim\limits_{n\to\infty} \dfrac{\log \phi_n}{\log n}$ exists.

From $y = (1 + (1/y))^n$, where $y \equiv \phi_n$ and $1 < y < n$, we have

$$\log y < \log n \quad \text{and} \quad \log \phi_n < \log n \quad \text{or} \quad \frac{\log \phi_n}{\log n} < 1 \text{ is bounded.}$$

For large n, also,

$$y = \left(1 + \frac{n/y}{n}\right)^n \lesssim e^{n/y} \quad \text{or} \quad \log y + \log\log y < \log n$$

or

$$\frac{\log y}{\log n} + \frac{\log\log y}{\log n} \lesssim 1.$$

It may be that $\log \phi_n / \log n$ is eventually monotonically increasing. A short computer program shows, however, that it is not monotone at first.

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