

A Kinetic Approach to the Random f -Graph Process with Nonuniform Edge Probabilities

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Starting with n labeled vertices and no edges, introduce edges, one at a time, so as to obtain a sequence of graphs each having no vertex of degree greater than f . The latter are called f -graphs. At each step the edge to be added is selected from among those edges whose addition would not violate the f -degree restriction and with probability proportional to the product of the respective numbers of available sites at the vertices of the potential edge. We call this procedure the *Random f -Graph Process with nonuniform edge probabilities (R*f-GP) of order n* . This is in contrast to the *Random f -Graph Process (Rf-GP) of order n* in which the edges that are added are selected with uniform probability. Using the *Law of Mass Action*, chemists have derived the degree distribution of the vertices in a graph generated by the R*f-GP. Here we apply a differential equation technique to obtain this degree distribution.

1. INTRODUCTION

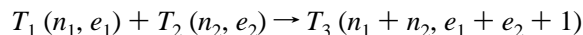
Starting with n labeled vertices and no edges, introduce edges, one at a time, so as to obtain a sequence of graphs each having no vertex of degree greater than f . The latter are called f -graphs. At each step the edge to be added is selected from among those edges whose addition would not violate the f -degree restriction and with probability proportional to the product of the respective numbers of available sites at the vertices of the potential edge. We call this procedure the *Random f -Graph Process with nonuniform edge probabilities (R*f-GP) of order n* . This is in contrast to the *Random f -Graph Process (Rf-GP) of order n* in which the edges that are added are selected with uniform probability (see ref 1).

The Rf-GP has as a special case the classic Erdős-Rényi *Random Graph Process*, this being the case $f = n - 1$. The bounded degree restriction $f < n - 1$ introduces difficulties of a type different than those encountered in the Random Graph Process. The interest in random graphs with bounded degree and in particular in the context of the Rf-GP and R*f-GP follows from their natural occurrence in network reliability theory and in chemistry and physics applications.^{1,2} The R*f-GP is related to chemical applications in the sense that the nonuniform edge probability reflects the condition that a vertex of lower degree emanates a greater attraction for bonding. Many of the questions posed in these models are the same, for example, those related to evolution such as hitting times and structure properties of the random graphs at various points in the evolution. As described in ref 1, there are many unresolved questions concerning the Rf-GP. This is also the case for the R*f-GP. In refs 3 and 4 we showed how a particular differential equation technique can

be used to obtain the asymptotic degree distribution for a random graph generated by the Rf-GP. The results are valid for any step in the Rf-GP for which the asymptotic proportion of vertices of degree f is not unity. Using the *Law of Mass Action*, chemists have derived the degree distribution of the vertices in a graph generated by the R*f-GP. Here we apply the method used in ref 3 to obtain this degree distribution.

2. LAW OF MASS ACTION

In physics, the Rf-GP provides a model for aggregation (coagulation), while the R*f-GP (for graphs of large order) models chemical polymerization processes. Both types of processes have been studied by physicists and chemists using various techniques to obtain information on the distribution of orders (aggregates, polymer molecules) and of vertex degrees of f -trees. Some results, identical with those obtained in this and previous work have been derived by making use of the *Law of Mass Action (LMA)*. This empirical law, due to Guldberg and Waage, describes the (statistical) rules governing formation and vanishing of species in chemical processes.⁵ In short, if one considers the random process of an edge introduction as chemists usually do



where $T_i(n_i, e_i)$ denotes an f -tree of order n_i and size $e_i = n_i - 1$. Then one of the results of the LMA is the *kinetic differential rate equation* having the form

$$\frac{dN_{T_3}}{dt} = kN_{T_1}N_{T_2}$$

Here the N_{T_i} 's denote the numbers of f -trees of order n_i in the (large) graph, while the k and t are positive parameters that chemists usually establish experimentally, the t having the notion of time. Detailed LMA based analysis leads to the conclusion that k should be proportional to

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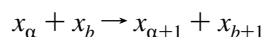
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$n_1 n_2$ for Rf-GP

$[n_1(f-2) + 2] [n_2(f-2) + 2]$ for R*f-GP

Another way that the LMA can be applied is in the analysis of the proportions x_d of vertices of a given degree d as they change in the R*f-GP. For the *chemical reaction* (here an edge is introduced at random) between vertices of degree α and β ($\alpha, \beta < f$) written as



the LMA kinetic rate equations are⁶

$$\frac{dx_0}{dt} = -\kappa_0 f x_0 \sum_{j=0}^{f-1} \kappa_j (f-j) x_j$$

and for $0 < d \leq f$

$$\frac{dx_d}{dt} = [\kappa_{d-1}(f-d+1)x_{d-1} - \kappa_d(f-d)x_d] \sum_{j=0}^{f-1} \kappa_j (f-j) x_j$$

For the R*f-GP all constants κ_α are equal and are usually made unity by rescaling the time units. However, in chemistry this is not a general rule. Note that if $\kappa_\alpha = 1/(f - \alpha)$ we recover equations equivalent to the kinetic differential equations for the Rf-GP derived in refs 3 and 4.

3. DERIVATION OF EQUATIONS

In the R*f-GP, let a graph G_s have degree distribution (X_0, X_1, \dots, X_f) where G_s is at level s (s = number of edges), has order n , and X_i (a function of s) is the number of vertices of degree i in G_s . We shall derive differential equations for the proportions (relative to n) of the X_i 's. At a crucial step in this derivation we shall, as in previous work,³ replace $\Delta X = X(s+1) - X(s)$, the change in X as s goes from s to $s+1$, by the expected change $E(\Delta X) = \sum \delta P(\Delta X = \delta)$.

Let

$$S = \sum_{i=0}^{f-1} (f-i) X_i$$

that is, S is the total number of available sites in G_s . Next, let

$$S^* = S/n$$

so that

$$S^* = \sum_{i=0}^{f-1} (f-i) x_i$$

, where $x_i = X_i/n$. Also, let

$$t = s/(fn/2) = 2s/fn$$

Lemma 3.1. If

$$x_i(t) = X_i(t)/n \quad \text{for } i = 0, 1, \dots, f, \quad S^*(t) = \sum_{i=0}^{f-1} (f-i) x_i(t)$$

and t is such that

$$\lim_{n \rightarrow \infty} S^*(t) > 0 \text{ a.s.}$$

then

$$\frac{dx_0}{d\tau} = -f x_0 S^*$$

and

$$\frac{dx_i}{d\tau} = -[(f-i)x_i - (f-i+1)x_{i-1}]S^* \quad \text{for } i = 1, 2, \dots, f-1$$

where

$$\tau = \frac{t}{f(1-t)}, \quad x_0(t)|_{t=0} = 1$$

$$x_i(t)|_{t=0} = 0 \quad \text{for } i = 1, 2, \dots, f-1$$

and

$$x_j(t) = 1 - \sum_{i=0}^{f-1} x_i(t)$$

Theorem 3.1. The solution to the system of differential equations of Lemma 3.1 is

$$x_i(\tau) = \binom{f}{i} (1-t)^{f-i} t^i \quad \text{for } i = 0, 1, \dots, f \quad (0 \leq t < 1)$$

with

$$t = \frac{f\tau}{1+f\tau}$$

Proof of Lemma 3.1. Let $a = 2s/fn$ be fixed, that is, $s = afn/2$. Then

$$\left. \frac{dx_0}{dt} \right|_{t=a} = \lim_{n \rightarrow \infty} \frac{x_0(a + 2/fn) - x_0(a)}{2/fn}$$

$$= \lim_{n \rightarrow \infty} (fn/2)(x_0((2s/fn) + (2/fn)) - x_0(2s/fn))$$

$$= \lim_{n \rightarrow \infty} (f/2)(X_0(s+1) - X_0(s))$$

The latter step follows from $nx_i(t) = X_i(t) = X_i(2s/fn) = X_i(s)$.

We now replace $X_0(s+1) - X_0(s)$ by its expected value. Note that where there is little chance of misinterpretation we have suppressed the display of the variables s and t so as to simplify the notation.

$$\begin{aligned} \left. \frac{dx_0}{dt} \right|_{t=a} &= \lim_{n \rightarrow \infty} (f/2) \left(-2 \binom{f^2(X_0)}{2} - \left(\frac{\sum_{i=1}^{f-1} f X_0(f-i) X_i}{D} \right) \right) \\ &= \lim_{n \rightarrow \infty} (f/2) \left(\frac{-f^2 X_0(X_0-1) - f X_0(S-X_0f)}{D} \right) \end{aligned}$$

$$= \lim_{n \rightarrow \infty} (f/2) \left(\frac{-f X_0 S + f^2 X_0}{D} \right)$$

$$= (f/2) \left(\frac{-f X_0 S}{D} \right)$$

where

$$D = \frac{1}{2} \sum_{0 \leq i, j \leq f-1} (f-i)(f-j) X_i X_j - \frac{1}{2} \sum_{0 \leq i, j \leq f-1} (f-i)(f-j) a_{ij}$$

with a_{ij} = the number of edges in G_s whose two vertices have degree i and j , respectively. Division of $X_0 S$ and D by n^2 yields

$$\frac{X_0 S}{D} = \frac{x_0 S^*}{D^*}$$

Therefore,

$$\left. \frac{dx_0}{dt} \right|_{t=a} = (f/2) \left(\frac{-f x_0 S^*}{D^*} \right)$$

Let

$$\tau = \frac{t}{f(1-t)}$$

Since $2D^* = (S^*)^2 = (f(1-t))^2$, when the a_{ij} terms in D^* are dropped, we arrive at

$$d\tau = \frac{f dt}{2D^*}$$

Thus,

$$dx_0 = (f/2) \left(\frac{-f x_0 S^*}{D^*} \right) dt$$

yields $dx_0 = -f x_0 S^* d\tau$. Thereby, obtaining

$$\frac{dx_0}{d\tau} = -f x_0 S^*$$

For the derivative of x_i we proceed as follows

$$\left. \frac{dx_i}{dt} \right|_{t=a} = \lim_{n \rightarrow \infty} \frac{x_i(a+2/fn) - x_i(a)}{2/fn}$$

$$= \lim_{n \rightarrow \infty} (f/2) (X_i(s+1) - X_i(s))$$

As above we replace $X_i(s+1) - X_i(s)$ by its expected value, that is

$$\left. \frac{dx_i}{dt} \right|_{t=a} = \lim_{n \rightarrow \infty} (f/2) E(\Delta X_i) \quad (3.1)$$

$$E(\Delta X_i) = -2P(\Delta X_i = -2) - P(\Delta X_i = -1) + P(\Delta X_i = 1) + 2P(\Delta X_i = 2)$$

for $i = 1, 2, \dots, f-1$. Thus

$$E(\Delta X_i) = -2 \left(\frac{(f-i)^2 \binom{X_i}{2} - a_{ii}}{D} \right) -$$

$$\left(\frac{\sum_{j=0, j \neq i}^{f-1} (f-i) X_i (f-j) (X_j - a_{ij})}{D} \right) +$$

$$\left(\frac{\sum_{j=0, j \neq i-1}^{f-1} (f-i+1) X_{i-1} (f-j) (X_j - a_{i-1,j})}{D} \right) +$$

$$2 \left(\frac{(f-i+1)^2 \binom{X_{i-1}}{2} - a_{i-1,i-1}}{D} \right)$$

Collecting only quadratic X terms in $E(\Delta X_i)$, where in particular here we have

$$D = \frac{1}{2} \sum_{0 \leq i, j \leq f-1} (f-i)(f-j) X_i X_j$$

we obtain

$$E(\Delta X_i) = -2 \left(\frac{(f-i)^2 X_i^2}{2D} \right) - \left(\frac{\sum_{j=0, j \neq i}^{f-1} (f-i)(f-j) X_i X_j}{D} \right) +$$

$$\left(\frac{\sum_{j=0, j \neq i-1}^{f-1} (f-i+1)(f-j) X_{i-1} X_j}{D} \right) + 2 \left(\frac{(f-i+1)^2 X_{i-1}^2}{2D} \right)$$

Continuing the computation of $E(\Delta X_i)$ we have

$$E(\Delta X_i) = \frac{((f-i+1)X_{i-1})^2}{D} - \frac{((f-i)X_i)^2}{D} +$$

$$\frac{(f-i+1)X_{i-1} \sum_{j=0, j \neq i-1}^{f-1} (f-j) X_j}{D} - \frac{(f-i)X_i \sum_{j=0, j \neq i}^{f-1} (f-j) X_j}{D} =$$

$$\frac{((f-i+1)X_{i-1})^2 - ((f-i)X_i)^2}{D} +$$

$$\frac{(f-i+1)X_{i-1}(S - (f-i+1)X_{i-1})}{D} -$$

$$\frac{(f-i)X_i(S - (f-i)X_i)}{D} = \left(\frac{(f-i+1)X_{i-1} - (f-i)X_i}{D} \right) S$$

Thus, since only quadratic terms in $E(\Delta X_i)$ have been retained (see (3.1)), we have

$$\left. \frac{dx_i}{dt} \right|_{t=a} = \lim_{n \rightarrow \infty} (f/2) \left(\frac{(f-i+1)X_{i-1} - (f-i)X_i}{D} \right) S$$

$$= (f/2) \left(\frac{(f-i+1)X_{i-1} - (f-i)X_i}{D} \right) S$$

We rewrite this expression by dividing numerator and

denominator by n^2 so that

$$\frac{dx_i}{dt} = (f/2) \left(\frac{(f-i+1)x_{i-1} - (f-i)x_i}{D^*} \right) S^*$$

where

$$D^* = \frac{1}{2} \sum_{0 \leq i, j \leq f-1} (f-i)(f-j)x_i x_j$$

As before, we let

$$d\tau = \frac{f dt}{2D^*}$$

to obtain

$$\frac{dx_i}{d\tau} = -[(f-i)x_i - (f-i+1)x_{i-1}]S^* \quad \text{for } i = 1, 2, \dots, f-1$$

By definition

$$x_f(t) = 1 - \sum_{i=0}^{f-1} x_i(t)$$

Proof of Theorem 3.1. Straightforward differentiation of

$$x_i(\tau) = \binom{f}{i} (1-t)^{f-i} t^i \quad \text{for } i = 0, 1, \dots, f \quad (0 \leq t < 1)$$

with

$$t = \frac{f\tau}{1 + f\tau}$$

together with the use of

$$S^* = f(1-t)$$

and

$$\frac{dt}{d\tau} = \frac{f}{(1 + f\tau)^2} = f(1-t)^2$$

shows that $x_i(\tau)$ satisfies the differential equations of Lemma 3.1.

4. CONCLUDING REMARKS

A few remarks concerning the chemical/physical interest in degree distributions are in order here. It has been known for some time that the degree distribution of a system is basic in polymerization reactions. In particular, in stepwise polymerization one can deduce size distribution information

of polymer species and design composition of systems from the degree distribution. This is applied in real systems to induce or avoid gelation. The latter being the polymer analogue of the threshold point at which a giant component appears in a random graph theoretical model. In real world applications this is used in the design of paints, resins, and plastics. The importance to life processes of this gelation transition and the corresponding species structure around this point was noted in ref 8 with the assertion that most of life exists in a narrow interval containing this transition. A few bonds more or less would make a species too stiff or too fluid to survive. Detailed overviews and extensive references concerning the relation of random graph models to physical systems can be found in refs 9–12.

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