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Random Sequential Adsorption on Random Trees

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Abstract When gas molecules bind to a surface they may do so in such a way that the adsorption of one molecule inhibits the arrival of others. Two models which have frequently been studied are the "dimer model" and the "blocking model", and rather complete solutions for these are known on fixed tree structures or Bethe lattices. In this paper comparisons are made between the occupation probabilities for vertices between fixed and random trees.

Keywords Interacting particle systems · Random sequential allocation · Dimer processes · Blocking models · Random graphs

1 Introduction

This paper is inspired by "Parking on a random tree" by Dehling, Fleurke and Kulske (DFK) [1]. They describe their problem as analogous to the Renyi parking problem, but it is closer to what are called Blocking models or hardcore models. There are two main types of models, those in which the molecules can leave and others be adsorbed onto the sites (see, for example, Gouet and Sudbury [3]), and those in which the molecules "stick". The latter models are designated as Random Sequential Adsorption. Fairly detailed analyses of these are given by Evans [2] in the physics literature and Penrose and Sudbury (PS) [4] in the mathematical literature. We shall follow the methods used in PS. In that paper they considered the processes on the infinite tree T_k, a graph in which each vertex is connected to $k+1$ other vertices. (Note: DFK consider graphs with k neighbours.) If a site is selected, and one bond is cut, then the site becomes the base of a rooted tree, R_k, which can be viewed as a branching system where each site leads to k further branches. A random rooted tree is a rooted tree in which the number of branches leading away from the root at each site is a set of independent random variables, each with probability generating function $G(s)$. The random rooted tree is thus also a representation of a Galton-Watson process. The random

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trees we shall consider will be such that, when a bond is cut at a site, the site becomes the base of a random rooted tree.

In the Blocking model particles arrive at each vertex at rate 1 and stick as long as none of the neighbouring vertices are occupied. At most one particle can occupy a vertex and no particles leave. Thus at each vertex there can only be one attempt for a particle to stick. If either the first succeeds or fails, no further particles can stick. Because of this, PS considers the case in which at each vertex there is a single arrival time which is uniformly distributed on $(0, 1)$. This simply makes the formulae easier to read for, whenever there is the function $1 - e^{-t}$ in the model with exponential arrival times, in the PS formulation there is t.

In the Dimer model pairs of particles arrive at neighbouring pairs of vertices independently and uniformly on $(0, 1)$ and stick if neither of the vertices is occupied. As in the Blocking model one has only to consider the first arrival.

Our main results are Theorems 1 and 2. The first part of Theorem 1 follows directly from the result in DFK, the second part using the relationship $G(s) > s^k$. The result is proved in Sect. 2. In Sect. 3 Theorem 3 gives sufficient conditions for a similar result for dimer processes. Section 4 gives a purely analytic argument for conditions to satisfy Theorem 3. The results are summarised in Theorem 2.

Theorem 1 *In the Blocking model, if, on random tree A the number of neighbours has p.g.f.* $sG_A(s)$, *and on random tree B the number of neighbours has p.g.f.* $sG_B(s)$ *and* $G_A(s) \geq G_B(s), 0 < s < 1$, *then the occupation probability of a vertex on A is greater for that on B at all* $0 < t \leq 1$. *In particular, among graphs with mean number of neighbours equal to* $k + 1$, *the occupation probability for a vertex is a minimum for* T_k, *the tree with a fixed number of neighbours.*

Although intuition is not always a good guide, one may imagine that the occupation probability is roughly related to 1/#*neighbours*, and, for positive random variables, $E(1/X) > 1/\mu_X$.

Theorem 2 *In the Dimer model on a random tree with the numbers of neighbours having mean* $k + 1$ *and p.g.f.* $sG(s)$, *the probability a pair of sites is occupied by a dimer is greater than for* T_k *if*

$$\int_{1/e}^{1} \frac{1}{G(s)} ds \geq 1,$$

or if the distribution corresponding to $G(s)$ *is geometric or Poisson.*

The probability a vertex is occupied is less than for T_k *if*

$$\int_{1/\sqrt{e}}^{1} \frac{1}{G(s)} ds \geq 1,$$

or if the distribution corresponding to $G(s)$ *is geometric or Poisson.*

Corollary 1 *The probability a pair is occupied by a dimer is greater on the random tree if every vertex has at least two neighbours.*

It may be possible to weaken the conditions for Theorem 2 as simulation of hundreds of thousands of distributions with powers up to $2k$ gave no counter-examples. However, the random probabilities were chosen in fairly simple ways (uniform, biased to high values of the random variable, low values, u-shaped etc.). They did not all satisfy the conditions of Theorem 2.

2 Single Vertices in the Blocking Model

The method used to treat this problem in PS is to first solve the problem on the rooted tree R_k (also known as the k-ary tree). On this graph the root (call it 0) has k neighbours and all other vertices have $k+1$. PS defines

$$\beta(t) = P(0 \text{ is unoccupied at time } t).$$

A change can only occur at 0 in $(t, t+dt)$ if the single particle which arrives there does so in that interval, and if all the neighbours of 0 are empty. But, given that 0 is unoccupied, the probability a neighbour is unoccupied is $\beta(t)$ and the events at each neighbour are independent. We thus have (32) of PS

$$\beta'(t) = -\beta^k \quad \Rightarrow \quad \beta(t) = [1 + (k-1)t]^{-1/(k-1)} \tag{1}$$

noting that $\beta(0) = 1$, since the graph is empty at time 0.

DFK treats the case of a random tree in which the number of neighbours at vertex i is $1 + X_i$ where the X_i are i.i.d.r.v.'s. Let $P(X_i = k) = g_k$, then X_i has p.g.f.

$$G(s) = \sum_{r=0}^{\infty} g_r s^r.$$

In the random case, the root has X_0 neighbours, and thus the left equation of (1) becomes

$$\beta'(t) = -\sum_{r=0}^{\infty} g_r \beta^r = -G(\beta) < -\beta^{\mu}, \tag{2}$$

since, for any r.v. X not constant a.s., Jensen's inequality implies $E[s^X] > s^{E(X)}$ or $G(s) > s^{\mu}$ where μ is the mean of X.

This is equivalent to equation (2.14) of DFK except that DFK has k neighbours where we have $k+1$. β is thus defined by the equation

$$\int_{\beta(t)}^{1} \frac{1}{G(s)} ds = t, \tag{3}$$

which is equivalent to equation (1.6) in DFK.

PS then defines $\alpha(t)$ to be the probability a vertex is unoccupied on the tree at time t so that

$$\alpha'(t) = -\sum_{r=0}^{\infty} g_r \beta^{r+1} = -\beta G(\beta) = \beta(t)\beta'(t)$$

using (2), which implies

$$\alpha(t) = \frac{1}{2}(1 + \beta^2(t)), \tag{4}$$

which is also true for the fixed tree T_k.

We now compare the tree T_k to the random tree in which each vertex has mean number of neighbours $k+1$. Define the corresponding β's to be β_k and β_X. Equations (1) and (2) imply that $\beta_k > \beta_X$. Since the occupation probability is $(1-\alpha^2)/2$ we have proved Theorem 1, since the argument for $G_A(s) > G_B(s)$ is the same.

There are some obvious cases which can be solved exactly.

1. *The Poisson distribution* We shall drop the subscript X. Equation (2) becomes

$$\beta' = -e^{k(\beta-1)} \quad \Rightarrow \quad \beta = 1 - \frac{1}{k}\ln(1+kt). \tag{5}$$

2. *The geometric distribution* Equation (2) becomes

$$\beta' = -\frac{1}{k+1-k\beta} \quad \Rightarrow \quad \beta = \frac{k+1-\sqrt{1+2kt}}{k}. \tag{6}$$

3. *The binomial distribution* Equation (2) becomes

$$\beta' = -\left(1 - \frac{k}{n}(1-\beta)\right)^n \quad \Rightarrow \quad \beta = 1 + \frac{n}{k}\left(\left(1 + k\frac{n-1}{n}t\right)^{-1/(n-1)} - 1\right). \tag{7}$$

3 Dimers

Consider the graph which is a rooted tree R_k (in which 0 is the root) plus the vertex -1 which is only connected to 0. Define

$$\beta(t) = P(-1 \text{ is unoccupied at time } t).$$

$\beta(0) = 1$, and the only way in which -1 can become occupied is when a dimer arrives at $-1, 0$. 0 is however the root of R_k and 0 is thus in the position of -1 k times over. As in the blocking model we define $\alpha(t)$ to be the probability a vertex is unoccupied in the dimer process on T_k. Now every vertex in T_k is in the position of -1 in the previous graph $k+1$ times over, giving us

$$\beta'(t) = -\beta^k \quad \Rightarrow \quad \beta(t) = [1+(k-1)t]^{-1/(k-1)}, \qquad \alpha(t) = \beta^{k+1}, \tag{8}$$

which is equivalent to equation (39) in PS. The corresponding equations in the random case are

$$\beta_X'(t) = -G(\beta_X), \qquad \alpha_X(t) = \beta_X G(\beta_X). \tag{9}$$

The situation is not so clear cut as in the blocking model. As before, $\beta > \beta_X$ but, because $G(s) > s^k, 0 < s < 1$, an inequality between α and α_X is not clear. A criterion for $\alpha < \alpha_X$ is given in Theorem 2, but it is believed true for a much wider class of distributions. Hundreds of thousands of p.g.f.'s with powers up to $2k$ were simulated and all gave this result. However, it is not true for all. With $G(s) = (1-k/n) + ks^n/n$ (9) implies $\beta_X(t) < 1-(1-k/n)t, \beta_X(1) < k/n$. At $t=1$ we are bound to have $\beta_X G(\beta_X) < \beta^{k+1}$ for large enough n.

A simple example which does work is the case $k=1, \beta = e^{-t}$ against the alternative $G(\beta_X) = (1+\beta_X)^2/4$. Equation (2) becomes

$$\beta_X' = -\frac{(1+\beta_X)^2}{4} \quad \Rightarrow \quad \beta_X = \frac{2-t}{2+t} \quad \Rightarrow \quad \beta_X G(\beta_X) = \frac{4(2-t)}{(2+t)^3} > e^{-2t}. \tag{10}$$

Now, consider the arrival of a dimer at a pair of sites. Define

$$\gamma(t) = P(\text{the pair is occupied by a dimer at time } t).$$

$\gamma(0) = 0$. For a dimer to arrive at time t requires that both ends are unoccupied. We thus have

$$\frac{d\gamma}{dt} = G^2(\beta_X(t)),$$

which implies that the occupation probability for a dimer is greater in the random case if $G(\beta_X(t)) > \beta(t)$.

Theorem 3 *If $\beta_X(t)G(\beta_X(t)) > \beta(t)^{k+1}$ then the probability a vertex is occupied by a dimer is less on the random tree. If $G(\beta_X(t)) > \beta(t)^k$ then the probability a pair of vertices is occupied by a dimer is greater on the random tree.*

4 Analysis of Differential Equations Arising in the Dimer Model

What follows is analytic rather than probabilistic. β now replaces what was β_X, b replaces β. The main result is Theorem 4 which is needed in conjunction with Theorem 3 to derive Theorem 2. At the end of the section we show that the Poisson and geometric distributions satisfy the third claim in Theorem 4.

Consider the two equations

$$\frac{d\beta}{dt} = -G(\beta), \qquad \frac{db}{dt} = -b^k, \quad 0 < t < 1, \tag{11}$$

where $G(.)$ is a p.g.f. with mean k and $\beta(0) = 1, b(0) = 1$. We shall show

Theorem 4 *For* $0 < t < 1$

1. $\beta(t) < b(t)$,
2. $G(\beta(t)) > b(t)^k$ *if* $G'(s) < kG^{(k-1)/k}(s), \beta(1) < s < 1$,
3. $\beta G(\beta(t)) > b(t)^{k+1}$, *if* $H'(s) < (k+1)sH^{(k-1)/(k+1)}(s), \beta(1) < s < 1$, *where* $H(s) = sG(s)$.

Proof Part 1 of Theorem 4 follows from the fact that $G(s) > s^k, 0 < s < 1$. Equations (11) are equivalent to

$$\int_{\beta(t)}^{1} \frac{1}{G(s)} ds = t = \int_{b(t)}^{1} \frac{1}{s^k} ds. \tag{12}$$

Put $y = G(s), z = s^k$ to obtain

$$\int_{G(\beta(t))}^{1} \frac{1}{yG'(G^{-1}(y))} dy = t = \int_{b^k(t)}^{1} \frac{1}{zkz^{(k-1)/k}} dz. \tag{13}$$

Thus, a sufficient condition for $G(\beta(t)) > b(t)^k$ is $G'(G^{-1}(y)) \le ky^{(k-1)/k}$ from which the second proposition in the theorem follows, since $G(.)$ is monotone. The third part follows in a similar manner to the second, this time putting $y = sG(s), z = s^{k+1}$. □

Lemma 5 *If $G(s)=ps^m+qs^{m+r}, m\geq 0, p+q=1, m+qr=k$ then $s\geq 1/e$ is a sufficient condition for $G'(s)<kG^{(k-1)/k}(s)$.*

Proof

$$\begin{aligned}G'(s)<kG^{(k-1)/k}(s) \quad &\Leftrightarrow \quad \left[\frac{G'(s)}{kG(s)}\right]^k<\frac{1}{G(s)}\\ &\Leftrightarrow \quad \left[\frac{pm+q(m+r)s^r}{k(p+qs^r)}\right]^k<\frac{s^k}{ps^m+qs^{m+r}}\\ &\Leftrightarrow \quad \left[1-\frac{rpq(1-s^r)}{k(p+qs^r)}\right]^k<\frac{s^{rq}}{p+qs^r}.\end{aligned}$$

Since $(1-a/k)^k\uparrow e^{-a}$

$$\exp\left\{-\frac{rpq(1-s^r)}{p+qs^r}\right\}\leq\frac{s^{rq}}{p+qs^r} \tag{14}$$

is a sufficient condition for $G'(s)<kG^{(k-1)/k}(s)$. Taking logarithms and rearranging, (14) is equivalent to

$$rpq(1-s^r)+(p+qs^r)[rq\ln(s)-\ln(p+qs^r)]\geq 0.$$

The l.h.s. equals 0 for $p=1, q=0$ and for $p=0, q=1$. The second derivative of the l.h.s. w.r.t. q equals

$$-2r(1+\ln(s))(1-s^r)-\frac{(1-s^r)^2}{1-q(1-s^r)},$$

which is ≤ 0 for $\ln(s)+1\geq 0$ from which the lemma follows. □

Lemma 6 *If $H(s)=ps^m+qs^{m+r}, m\geq 1, p+q=1, m+qr=k+1$ then $s>1/\sqrt{e}$ is a sufficient condition for $H'(s)<(k+1)sH^{(k-1)/(k+1)}(s)$.*

Proof The condition above is equivalent to

$$\begin{aligned}\left[\frac{H'(s)}{(k+1)sH(s)}\right]^{k+1}<\frac{1}{H^2(s)} \quad &\Leftrightarrow \quad \left[\frac{pm+q(m+r)s^r}{(k+1)(p+qs^r)}\right]^{k+1}<\frac{s^{2qr}}{(p+qs^r)^2}\\ &\Leftrightarrow \quad \left[1-\frac{rpq(1-s^r)}{(k+1)(p+qs^r)}\right]^{k+1}<\frac{s^{2rq}}{(p+qs^r)^2}.\end{aligned}$$

Since $(1-a/k)^k\uparrow e^{-a}$

$$\exp\left\{-\frac{rpq(1-s^r)+1}{(p+qs^r)}\right\}\leq\frac{s^{2rq}}{(p+qs^r)^2}. \tag{15}$$

is a sufficient condition for $[\frac{H'}{(k+1)s}]^{k+1}<H^{k-1}(y)$. Taking logarithms and rearranging, (15) is equivalent to

$$rpq(1-s^r)+(p+qs^r)[2rq\ln(s)-2\ln(p+qs^r)]\geq 0.$$

The l.h.s. equals 0 for $p = 1, q = 0$ and for $p = 0, q = 1$. The second derivative of the l.h.s. w.r.t. q equals

$$-2r(2\ln(s)+1)(1-s^r) - \frac{2(1-s^r)^2}{1-q(1-s^r)},$$

which is ≤ 0 for $2\ln(s)+1 \geq 0$ from which the lemma follows. □

We have shown that the conditions for Theorem 4 apply for all p.g.f.'s concentrated on two points. We now wish to extend this to all p.g.f.'s with mean k.

Lemma 7 *Every finite p.g.f. mean k can be expressed as a mixture of p.g.f.'s with mean k concentrated on two values.*

Proof Consider the p.g.f. $\sum_{i=0}^{N} a_i x^i$, $\sum i a_i = k$. Let m, n be the minimum and maximum i s.t. $a_i \neq 0$. Since $m < k < n$ there exists $0 < p < 1$ s.t. $pm + (1-p)n = k$ so that $px^m + (1-p)x^n$ is a p.g.f. with mean k. First, suppose that

$$a_m \leq p(a_m + a_n) \quad \Leftrightarrow \quad \frac{1-p}{p} a_m \leq a_n,$$

then

$$\sum_{i=0}^{N} a_i x^i = \frac{a_m}{p}(px^m + (1-p)x^n) + bx^n + \sum_{i=m+1}^{n-1} a_i x^i$$

where $a_m/p \leq 1, b \geq 0$. If $a_m > p(a_m + a_n)$ then the higher power is removed. We now apply the same process to $bx^n + \sum_{i=m+1}^{n-1} a_i x^i$ until the original p.g.f. is a mixture of two-value p.g.f.'s. □

Lemma 8 *If $G_1, \ldots, G_m$ satisfy $G_i'(s) < kG_i^{(k-1)/k}(s)$ then so does $\sum_{i=1}^{m} p_i G_i$. A similar result holds for $H'(s) < (k+1)sH^{(k-1)/(k+1)}(s)$.*

Proof This follows from Jensen's inequality. Since $x^{(k-1)/k}$ is concave for $0 < x < 1$ we have $\sum p_i x_i^{(k-1)/k} \leq (\sum p_i x_i)^{(k-1)/k}$. Similarly for the power $(k-1)/(k+1)$. □

Lemma 9 *Every p.g.f. $G(s)$, mean k, satisfies $G'(s) < kG^{(k-1)/k}(s)$ for $s > 1/e$ and $G + sG'(s) < (k+1)s^{2k/(k+1)}G^{(k-1)/(k+1)}(s)$ for $s > 1/\sqrt{e}$.*

Proof Lemmas 5–8 imply the lemma is true for every finite p.g.f. Since, for any fixed s, any p.g.f. can be arbitrarily closely approximated by a sequence of finite p.g.f.'s, the theorem is also true for all p.g.f.'s. □

We can now prove most of Theorem 2. We note that if

$$\int_{1/e}^{1} \frac{1}{G(s)} ds \geq 1,$$

then any inequality true for $s > 1/e$ will be true for $s > \beta(1)$. We then apply Lemma 9, Theorems 3 and 4. Further, if $G(0) = 0$, which is equivalent to every vertex being attached to at least 2 other vertices, then $G(s) < s, 0 < s < 1$ and the above integral condition will be satisfied.

Finally, we show that the third condition of Theorem 4 applies to both the geometric and the Poisson distributions. For $G(s) = e^{k(s-1)}$,

$$\left[\frac{H'(s)}{(k+1)sH(s)}\right]^{k+1} < \frac{1}{H^2(s)} \quad \Leftrightarrow \quad p(s) = \left(\frac{e^{s-1}}{s}\right)^{2k}\left(\frac{1+ks}{1+k}\right) \leq 1.$$

It follows that

$$\frac{p'(s)}{p(s)} = \frac{2ks^2 - (k-3)s - 2}{s(1+ks)}.$$

$p'(0) < 0$, $p'(1) > 0$, and, since the numerator is quadratic, $p(s)$ decreases from ∞ to a minimum before increasing to 1. Thus, if $p(s_0) < 1, 0 < s_0 < 1$ then $p(s) \leq 1, s_0 \leq s \leq 1$. Therefore we only need to test the above inequality above for $\beta(1) = 1 - \ln(k+1)/k$.

It is simple to check the inequality for $k = 1$. For $k > 1$, $1 + \ln(1+k)/k > 0.5$, and we check the inequality at 0.5. $(e^{-5}/0.5)^2 = 1.47$ and the ratio of $[(1+k/2)/(1+k)]^{k+1}$ to the preceding term is $< 2/3$ and thus the inequality holds for all k.

For $G(s) = 1/(k+1-ks)$,

$$\left[\frac{H'(s)}{(k+1)sH(s)}\right]^{k+1} < \frac{1}{H^2(s)} \quad \Leftrightarrow \quad p(s) = (k+1-ks)^{k+3}s^{2k} \geq 1.$$

$p(1) = 1$, $p'(s) < 0, s > 2/3$, $p'(s) > 0, s > 2/3$ and thus we only check the inequality at $s = \beta(1) = (k+1-\sqrt{1+2k})/k$. This is simple to check for $k = 2, 3, 4, 5, 6$. For $k \geq 4$, $\beta(1) \geq 0.5$ and $p(0.5) = (k+2)^{k+3}(0.5)^{3k+3}$. For $k \geq 6$ this is clearly increasing as $(k+2)(0.5)^3 \geq 1$.

Since $\beta > b$, it is clear that $\beta G(\beta(t)) > b(t)^{k+1} \Rightarrow G(\beta(t)) > b(t)^k$ so that we do not need to check the geometric and Poisson for the latter.

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