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Radial Heat Diffusion from the Root of a Homogeneous Tree and the Combinatorics of Paths

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Abstract. – *We compute recursively the heat semigroup in a rooted homogeneous tree for the diffusion with radial (with respect to the root) but non-isotropic transition probabilities. This is the discrete analogue of the heat operator on the disc given by* $\Delta + c\,\dfrac{\partial}{\partial r}$ *for some constant c that represents a drift towards (or away from) the origin.*

1. – Introduction.

Consider an infinite homogeneous tree, regard its edges as thermal conductors, and assign a temperature distribution on its vertices at time zero. Several papers have considered the heat diffusion at later times. Because of the discrete nature of the environment, it is natural to limit attention to discrete consecutive time intervals. The explicit solution of the heat equation on a homogeneous tree equipped with an isotropic nearest neighbor transition operator (the generator of the heat semigroup) was obtained in [6] in the form of a computable non-recursive formula which is not an explicit closed formula because it contains a summation term (the analogue of an integral over time in the continuous setup). The same expression is derived in [2] by a different approach (the inversion formula for the Radon transform). Estimates for the heat maximal functions (the maximum temperature) for the isotropic nearest neighbor operator are in [7]. For this operator, the asymptotics of the heat semigroup had been studied previously in the context of the local central limit theorem in [9] and [8]. The same problem was solved in [4] for nearest neighbor anisotropic transition operators, and in [5] for finitely supported operators: these are the first instances where anisotropic heat semigroups are considered (some related probabilistic topics are considered in [10]).

Here we deal with the case of a homogeneous tree with a fixed vertex as root, equipped with a nearest neighbor transition operator that is isotropic only forward, but may have a radial drift towards or away from the root. In particular, our transition operator depends on the choice of the root.

The expression of the heat semigroup given in this paper, being recursive instead of in closed form, may not be directly applicable to computational questions, but its proof is remarkably different from the previous approaches: it is an interesting use of combinatorics on paths.

More precisely, let T be homogeneous tree of degree $q+1$ rooted at a vertex e. Let $p \in (0,1)$ and set $r = 1-p$. We consider a transition operator P on the vertices of T with probabilities $P(u,v)$ as follows:

$$
\begin{aligned}
&P(e,v) = \frac{1}{q+1}, && \text{if } |v| = 1 \\
&P(v,v^-) = r, && \text{if } v \neq e \\
&P(v^-,v) = \frac{p}{q}, && \text{if } v \neq e
\end{aligned}
\tag{1}
$$

where $|v| = n$ is the distance betweeen v and e, and if $v \neq e$ we denote by v^- the predecessor of v (that is, its neighbor closest to e).

P acts on functions on the tree by the rule $Pg(v) = \sum P(v,w)g(w)$. We wish to study its k-th iterate P^k, that is, the transition operator with kernel $P^k(v,w)$ given by the k-th power of the matrix $P(v,w)$. In particular, for f a radial function, we wish to calculate $P^k f$. Radial functions may be considered as functions on $\mathbb{N} = \{0,1,2,...\}$. Since the forward probabilities are isotropic, the action of P on radial functions is the same as the action of the radialized operator μ on functions on the natural numbers. In this reduction to $\mathbb{N}$ the transition probabilities change to

$$
\mu(0,1) = 1 \qquad \mu(n,n+1) = p \quad \text{for} \quad n > 0 \qquad \text{and} \qquad \mu(n+1,n) = r. \tag{2}
$$

(As expected: when a path visits 0, the next step is necessarily to 1).

After this radial reduction, $\mu^k f(n)$ becomes a linear combination of $f(s)$ where $n+k-s$ is even. That is:

$$
\mu^k f(n) = \sum_{t=0}^{k} C_{n,k,t} f(n+k-2t)\,. \tag{3}
$$

In particular, if – by abuse of notation – we write $\mu^k = \mu^k \delta_0$, then

$$
\mu^k(n) = \begin{cases} C_{n,k,(n+k)/2} & \text{if } \ n+k \text{ is even} \\ 0 & \text{if } n+k \text{ is odd} \end{cases}
$$

It is worth observing the relation between $\mu^k(n)$ and the row by column action of the n-th iterate μ^n of the transition operator μ. Denote by $\mu^k(v,w)$ the matrix coefficient of the k-th iterate of the transition operator on $\mathbb{N}$ obtained by radializing P. Then one has:

$$
\begin{aligned}
\mu^k f(n) = \sum_{j=0}^{\infty} \mu^k(n,j) f(j) &= \sum_{n-k \le j \le n+k} \mu^k(n,j) f(j) \\
&= \sum_{t=0}^{k} C_{n,k,t} f(n+k-2t)\,,
\end{aligned}
$$

where $C_{n,k,t}$ is the number of paths from n to $N = n + k - 2t$ of length k, each weighted with its probability. Therefore

$$P^k f(v) = \sum_{t=0}^{k} C_{|v|,k,t} f(|v| + k - 2t)\,,$$

where $k - 2t$ is the distance between $|v|$ and $|w|$.

There are many more paths in the tree that connect v and w than paths from $|v|$ to $|w|$ on $\mathbb{N}$, but when we sum over all such paths the respective probability weighted contributions $C_{n,k,t}$ and $C_{|v|,k,t}$ are the same, thanks to (1) and (2).

For example, if $n > k$, then

$$\mu^k f(n) = \sum_{t=0}^{k} \binom{k}{t} p^{k-t} r^t f(n + k - 2t)$$

where t is the number of backward steps in the paths of length k in $\mathbb{N}$ that start at n. This yields the value $C_{n,k,t} = \binom{k}{t} p^{k-t} r^t$ for $n > k$, that is for the paths that are too short to return to 0, but unfortunately not for the longer path (see the comments at the end of this Section). In the rest of the paper we compute $C_{n,k,t}$ in many other cases. Just counting the arbitrarily long paths that do not reach 0 turns out to be considerably more complicated (Lemma 2.1 below). Let us compute the recurrence relations satisfied by these coefficients.

The function μ satisfies the following rules:

$$\begin{aligned}
&\mu^0 f(n) = f(n)\,,\\
&\mu f(0) = f(1)\,,\\
&\mu f(n) = p f(n+1) + r f(n-1) \qquad \text{for } n \geq 1\,.
\end{aligned}$$

Therefore

$$\begin{aligned}
&C_{n,0,t} = \delta_{0,t}\,,\\
&C_{0,1,t} = \delta_{0,t}\,,\\
&C_{n,1,t} = p\delta_{0,t} + r\delta_{1,t} \qquad \text{for } n \geq 1\,.
\end{aligned}$$

Thus

$$\mu^{k+1} f(0) = \mu^k f(1),$$

$$\text{and, for } n \geq 1, \qquad \mu^{k+1} f(n) = p\mu^k f(n+1) + r\mu^k f(n-1)\,, \tag{4}$$

or equivalently

$$C_{0,k+1,t} = C_{1,k,t},$$

$$\text{and, for } n \geq 1, \qquad C_{n,k+1,t} = pC_{n+1,k,t} + rC_{n-1,k,t-1}\,.$$

(the last identity follows from (4) and (3), that yield

$$\sum_{t=0}^{k+1} C_{n,k+1,t}\, f(n+k+1-2t)$$
$$= \sum_{s=0}^{k} p\, C_{n+1,k,s}\, f(n+1+k-2s) + \sum_{h=0}^{k} r\, C_{n-1,k,h}\, f(n-1+k-2h)$$

for *every* function f).

We shall calculate the probabilities $C_{n,k,t}$ as follows: we need to find all the paths in $\mathbb{N}$ which start at n and end at $N = n+k-2t$ after k steps, calculate the probabilities of each path, and add them up.

There are two complications. First of all, all forward probabilities are the same *except* the probability of going from 0 to 1. Second, the functions are defined only on $\mathbb{N}$ and not on $\mathbb{Z}$, and so we cannot use simple group theoretic calculations to solve the problem.

2. – The graph of a path in the tree: Dyck paths.

A *Dyck path* of length k is the graph of a length k path in the integers with respect to time, assuming that the speed of motion along edges is 1 to go up and -1 to go down (actually, the speed is irrelevant for our approach). So a Dyck path is a piecewise linear graph whose segments have slope ± 1. We can as well restrict attention to the vertices of this piecewise linear curve: then the Dyck path becomes a finite sequence $(a, b_0), (a+1, b_1), \ldots, (a+k, b_k)$ in $\mathbb{Z} \times \mathbb{Z}$, where $b_{i+1} = b_i \pm 1$. With a path $c = [c_0, \ldots, c_k]$ from n to N, we associate the Dyck path

$$(0, n) = (0, c_0), (1, c_1), \ldots, (k, c_k) = (k, N).$$

We shall need the number of paths with certain properties: we compute this number in the following lemma, whose first part, taken from [3] (see also [1]), is a good model for the rest of the lemma and for some of the arguments in the rest of the paper.

From now on we denote by $\mathbb{Z}_+$ the positive integers. We say that a Dyck path that start at $(0, m)$ with $m > 0$ *never touches* 0 if it remains in $\mathbb{N} \times \mathbb{Z}_+$.

LEMMA 2.1. – (*i*) *The number of Dyck paths of length* $k = N - 1 + 2t$ *from* $(0, 1)$ *to* (k, N) *which never touch* 0 *is* $\dfrac{k+1-2t}{k+1-t}\dbinom{k}{t}$.

By reflection about the line $x = k/2$ the same formula also gives the number of Dyck paths from $(0, N)$ to $(k, 1)$ that never touch 0.

(*ii*) *For n, $N > 0$, the number of Dyck paths that go from $(0, n)$ to (k, N) without touching* 0 *is* 0 *if $k < |N - n|$, and*

$$\binom{k}{t} - \binom{k}{t-n}$$

otherwise.

PROOF. – The ascending paths in part (*i*) have length k and go up $N + t - 1$ times and down t times: clearly, there are $\binom{k}{t}$ paths of this type. We need to restrict attention to those paths that do not touch 0, that is, to exclude those who do. By the André reflection principle [3, pg. 72], the paths that touch 0 correspond bijectively to all (unrestricted) paths of length $k = N + 2t - 1$ from $(1, 0)$ to (k, N): to see this, simply reflect across the x-axis that part of the latter paths between $(0, -1)$ and the first point at which it touches the x-axis.

These paths cover an overall distance of $N + 1$ vertical steps, and since their length is $N + 2t - 1$ there are $t - 1$ *cancellations* (vertical steps repeated back and forth). Therefore these paths go up $N + t$ times and down $t - 1$ times, and so their number is $\binom{k}{t-1}$. Thus the number of paths in the statement is

$$\binom{k}{t} - \binom{k}{t-1} = \frac{k+1-2t}{k+1-t}\binom{k}{t}.$$

For part (*ii*), if a path goes from $n > 0$ to $N = n + k - 2t$ in k steps (and clearly we must have $k \geq N - n$), it must go $k - t$ steps in the direction from n to N and t in the opposite direction. That is, if $n \leq N$ such a path goes up $k - t$ times and down t times, and viceversa for $n > N$.

As a consequence, the number of all Dyck paths from $(0, n)$ to (k, N) without restriction, is $\binom{k}{t}$.

We now show that there are $\binom{k}{t-n}$ such paths that touch 0. By the André reflection principle, paths from n to N touching 0 correspond to arbitrary paths from $-n$ to N. Hence they must move up $n + k - t$ times and down $t - n$. So there are $\binom{k}{t-n}$ such paths, and so the total number of paths which do not touch 0 is the difference $\binom{k}{t} - \binom{k}{t-n}$. □

We now need the cardinalities of the sets of paths for (slightly) different beginning and end points. To make the paper more readable, we collect in the next statement the formulas needed later.

COROLLARY 2.1. – (i) [3] *The number of Dyck paths of length* $2n$ *from* 1 *to* 1 *which never touch* 0 *is the* n^{th} *Catalan number* $C_n = \dfrac{1}{n+1}\dbinom{2n}{n}$.

(ii) *The number of Dyck paths of length* $k-1 = N-1+2t$ *from* $(1,1)$ *to* (k,N) *which never touch* 0 *is* $\dfrac{k-2t}{k-t}\dbinom{k-1}{t}$. *This is also the number of Dyck paths that go:*

- *from* $(0,N)$ *to* $(k-1,1)$ *never hitting* 0;
- *from* 0 *to* N *in* $k = N+2t$ *steps again without hitting* 0;
- *from* N *to* 0 *in* $k = N+2t$ *without hitting* 0 *before the end.*

PROOF. – Part (i) and the first two claims of part (ii) come from Lemma 2.1(i), the former by setting $k = 2n, N = 1$, and $t = n$, and the latter by moving the whole Dyck path to the left by one, so that it goes from $(0,1)$ to $(k-1, N-1)$, or from $(k-1, N-1)$ to $(0,1)$. The third (resp. fourth) part is equivalent to the first (resp. second) by noting that the first (resp. last) step goes from 0 to 1 (resp. 1 to 0). □

In the rest of the paper, we split the computation of $C_{n,k,t}$ into the cases $n = 0$ and $n > 0$.

3. – Starting point $n = 0$.

In this section we compute the contribution of all the paths from 0 to N in, say, $k = N + 2t$ steps.

These paths must go up $N + t$ times and go down t times. Let us assume that the path touches 0 s times before reaching N (this includes the initial step but excludes the last hit if $N = 0$). All the up probabilities are p except for those starting at 0, which are 1, and all the down probabilities are r. Hence the probability for such a path is $p^{N+t-s}r^t$. It remains only to find out the number of such paths. In order to do this, we count the number of Dyck paths from $(0,0)$ to (k,N).

Let us first study the paths that go from 0 to 0 in $k = 2t$ steps without ever touching 0 in between. The associated probability is $p^{t-1}r^t$. Note that the first step is from 0 to 1 and the last from 1 to 0. Therefore these paths are in one to one correspondence with the paths of length $2n = 2t-2$ from 1 to 1 (or equivalently the Dyck paths from $(0,1)$ to $(2n,1)$) that remain in $\mathbb{N} \times \mathbb{Z}_+$. We have shown in part (i) of Corollary 2.1 that the number of these paths is the nth Catalan number C_n. Observe that the length of the path from 0 to 0 is $2n+2$. We recall that in our case $n = t-1$. So there are C_{t-1} paths that go from 0 to 0 in $2t$ steps without touching 0 in between.

Next we consider a path that goes from 0 to $N > 0$ in $k = N + 2t$ steps without touching 0 in between. The corresponding probability is $p^{N+t-1}r^t$ because we go up $N+t$ times (and only once from 0) and down t times. Since the first step is necessarily from 0 to 1, this corresponds to going from 1 to N in $k-1$ steps without touching 0. This corresponds to the Dyck paths from $(1,1)$ to (k,N) which remains in $\mathbb{N}\times\mathbb{Z}_+$. The number of such paths, computed in the first statement of part (*ii*) of Corollary 2.1, is $\dfrac{k-2t}{k-t}\dbinom{k-1}{t}$.

We are now ready to calculate $C_{0,k,t}$, that is, the probability of moving from 0 to $N=k-2t$ in k steps with t backward returns.

THEOREM 3.1. – *If $N=k-2t=0$, then*

$$C_{0,k,t}=C_{0,k,\frac{k}{2}}=\sum_{s=2}^{t+1}\sum_{m_1+\ldots+m_{s-1}=t-s+1}C_{m_1}C_{m_2}\ldots C_{m_{s-1}}\,p^{k-t-(s-1)}r^t,$$

while, if $N>0$, then

$$C_{0,k,t}=\frac{N}{N+t}\binom{N+2t-1}{t}p^{N+t}r^t$$

$$+\sum_{s=2}^{t+1}\sum_{m_1+\ldots+m_s=t-s+1}C_{m_1}C_{m_2}\ldots C_{m_{s-1}}\cdot\frac{N}{N+m_s}\binom{N+2m_s-1}{m_s}p^{N+t-s+1}r^t.$$

PROOF. – We deal first with the case $N>0$. The paths that we are considering reach N from 0 in $k=N+2t$ steps. Here t is the number of steps down, that is the number of backwards steps. There is a finite number s of visits to 0 before the end of the path (at least one, since the path starts at 0), but remember that now the path does not end at zero. In other words, there are $s-1$ consecutive subpaths from 0 to 0. Let $n_1,n_2,\ldots,n_{s-1}$ be the lengths of these subpaths, that is, the distance in time between consecutive visits to 0. That is, the path touches 0 at the steps $0,n_1,n_1+n_2,n_1+n_2+n_3,\ldots$. Each visit requests a step down (from 1 to 0), so $0\le s-1\le t$, that is, $1\le s\le t+1$.

The corresponding probability is $p^{N+t-s}r^t$. Each n_i is positive, and (since the subpath starts at 0) even. Set $m_i=(n_i-2)/2$: observe that $2m_i$ is the length of the subpath from 1 to 1 obtained by dropping the first and last segment from the path from the i-th visit to 0 to the $(i+1)$-th, and therefore m_i is the number of cancellations (backwards steps) of this subpath. By part (*i*) of Corollary 2.1, the number of paths that touch 0 between the $i-th$ and the $(i+1)-th$ such point is the Catalan number C_{m_i}. In addition, from the final 0 at time $n_1+n_2+\cdots+n_{s-1}$ we need to reach N in, say, $n_s=N+2m_s$ steps without touching 0 (here, again, m_s is the number of backward steps after the last visit to 0). We have shown in the third statement of part (*ii*) of Corollary 2.1 that the number of such paths is $\dfrac{n_s-2m_s}{n_s-m_s}\dbinom{n_s-1}{m_s}$, that is, $\dfrac{N}{N+m_s}\dbinom{N+2m_s-1}{m_s}$. Observe that, in the particular case $s = 1$, where the paths start at zero and never return there, one has

$$n_s \equiv n_1 = k \qquad \text{and} \qquad m_s = t\,. \tag{5}$$

Moreover, $\sum_{i=1}^{s-1} m_i$ is the sum of all backward steps until the last visit to 0 minus $s-1$ (because each such m_i is the number of backward steps in the subpath from 1 to 1, and so each time we miss the last backward step from 1 to 0). Therefore

$$\sum_{i=1}^{s-1} m_i = t - m_s - (s-1)\,, \tag{6}$$

since t is the total number of backward steps in the whole path, and m_s is the number of backward steps after the last return to 0 (remember that we are assuming that the last visit to 0 occurs before the end of the path). Identity (6) amounts to

$$\sum_{i=1}^{s} m_i = t - s + 1\,. \tag{7}$$

Now we split $C_{0,k,t}$ as the sum of the contribution of the paths that never return to zero (case $s = 1$) and those of the terms with $s > 1$ returns to zero. Remember that the number of returns to zero satisfies $s < t+1$ and $\sum_{i=1}^{s} m_i = t - s + 1$, whereas, if there is no such return, then $m_s = t$. This proves the first equality of the statement. The other equality in the statement follows from this because $n_s - 2m_s = N = k - 2t$, hence $k - t - s = N + t - s$.

Now it is easy to compute $C_{0,k,t}$ in general. It is sufficient to allow the end of the path to be 0. The only difference is that, if the path ends at 0, that is if $N = k - 2t = 0$, then it finishes after $n_1 + n_2 + \ldots + n_{s-1}$ steps, and we must omit the special contribution of the remaining last n_s steps considered in the previous part of the proof: that is, $n_s = 0$, hence $m_s = 0$. On the other hand, in this case we do not miss a factor p as a consequence of the last visit to zero (at time N), because there is no further jump from 0 to 1. Therefore in this case one has

$$\begin{aligned} C_{0,k,t} = C_{0,k,\frac{k}{2}} &= \sum_{s=2}^{t+1} \sum_{m_1+\ldots+m_{s-1}=t-s+1} C_{m_1} C_{m_2} \ldots C_{m_{s-1}} p^{k-t-(s-1)} r^t \\ &= \sum_{s=1}^{t} \sum_{m_1+\ldots+m_s=t-s} C_{m_1} C_{m_2} \ldots C_{m_s} p^{k-t-s} r^t\,. \end{aligned}$$

□

REMARK 3.1. – If $N = 0$, then the special term in Theorem 3.1,

$$\frac{N}{N+m_s} \binom{N+2m_s-1}{m_s}\,,$$

has value 1 because we are taking $m_s = 0$. This leads to a unified formulation of the two cases $N = 0$ and $N > 0$ in Theorem 3.1. Indeed, identity (7) yields

$$m_s = t - s + 1 - \sum_{i=1}^{s-1} m_i \,. \tag{8}$$

By defining m_s this way when $N > 0$ (and of course $m_s = 0$ otherwise), the last identity of Theorem 3.1 holds in both the cases $N = 0$ and $N > 0$, provided that the summation over $m_1, \ldots, m_{s-1}$ is understood to be zero when $s = 1$.

4. – Starting point $n > 0$.

In order to deal with the general case, we first compute the contribution of the paths that go from $n > 0$ to $N = n + k - 2t$ in k steps without touching 0 (here $k \geq |N - n|$). We have computed their number in part (*ii*) of Lemma 2.1. We recall from the proof of that lemma that, if $n \leq N$, these paths go up $k - t$ times and down t times. We shall limit attention to this case: the opposite case, $n > N$, is obtained by swapping the transition coefficients p and r. So, for $n < N$, the corresponding probability is thus $p^{k-t}r^t$, and by the lemma the total number of such paths is $\binom{k}{t} - \binom{k}{t-n}$.

Next we compute the contribution of those paths from n to N that touch 0, by counting how many times they hit 0. For each $i \geq 0$, we consider the paths that touch 0 for the first time after $n + 2i$ steps, and continue from there with a path going from 0 to N in $k - n - 2i$ steps. Here i is the number of backward steps (that is, steps up) in the beginning descent (the first subpath from n to 0), so $n + i$ is the number of steps down in the beginning path. In particular, $n + i$ cannot exceed the global number t of backward steps, that is $i \leq t - n$.

We have made both calculations previously: in part (*ii*) of Corollary 2.1 we have proved that this number is $\dfrac{n}{n+i}\dbinom{n+2i-1}{i}$. Observe that the reflection swaps the role of forward and backward probabilities: therefore the probability associated to the beginning path (first descent to 0) is $p^i r^{n+i}$. Next we determine the number of paths going from 0 to N in $k - n - 2i$ steps. The probability connected to this is exactly the number $C_{0,k-n-2i,t-n-i}$. Summing these contributions we reach the general result, that is, the expression for the powers of μ at all vertices, in the notation of Section 1:

THEOREM 4.1. – *Let* $n > 0$ *and* $N \geq 0$. *Let* $k = |N - n| + 2t$. *If* $n \leq N$,

$$C_{n,k,t} = \left[\binom{k}{t} - \binom{k}{t-n}\right] p^{k-t} r^t + \sum_{i=1}^{t-n} \frac{n}{n+i}\binom{n+2i-1}{i} C_{0,k-n-2i,t-n-i}\, p^i r^{n+i}.$$

If $n > N$ the same formula holds provided the coefficients p and r are interchanged in the first term of the right hand side.

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