

Branch Node Asymptotics and the Grand Partition Function

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Our next task is to apply our asymptotic techniques to our branch node counting series. These series had multivariate generating functions of the form

$$F(x, y) = \sum_{n=0}^{\infty} \sum_{b=0}^{\infty} F_{nb} x^n y^b \quad (1)$$

We wish to treat this generating function as a single variate generating function so we will consolidate the like terms of x to and rewrite equation 1 as:

$$F(x, y) = \sum_{n=0}^{\infty} \left(\sum_{b=0}^{\infty} F_{nb} y^b \right) x^n \quad (2)$$

To highlight this single variable quality we will rewrite our generating function using the following notations

$$F_y(x) \equiv \sum_{n=0}^{\infty} F_n(y) x^n = F(x, y) \quad (3)$$

$$F_n(y) \equiv \sum_{b=0}^{\infty} F_{nb} y^b \quad (4)$$

We can give some physical meaning to these new coefficients $F_n(y)$. First we note that $F_n(1) = F_n$ where F_n are the coefficients of the non-branch-node-counting series. We can begin to think of y as some sort of exponential weighting factor that is dependent on the number of branch nodes. It makes sense to interpret the value of y as the exponentiated energy that it takes to create a branch point. This energy is clearly the chemical potential of a branch point which we will call μ_b . Then we may make thermal interpretation of the value of y as the boltzmann weighted chemical potential which is a value called the fugacity.

$$y = e^{\frac{\mu_b}{k_B T}} \quad (5)$$

Clearly, $y=1$ corresponds to $\mu_b = 0$ meaning it takes no energy to create or remove a branch node which was an assumption we made when computing the partition function T_n . These new coefficients $F_n(y)$ are a generalization on our non-branch-counting partition function F_n . The number of branch nodes is not assumed to be fixed. Rather, we associate a chemical potential with the creation or destruction of a branch node. This means that $F_n(y)$ is a Grand Partition Function in terms of the number of branch points.

For convenience I will rewrite Theorem 1 here:

Theorem 1. *Let $H(x, y(x))$ be a complex valued function that is analytic in a neighborhood of $(x_0, G(x_0))$. If the following conditions are met:*

1. $H(x_0, G(x_0)) = 0$
2. $G(x)$ is analytic for $|x| < |x_0|$ where x_0 is the unique singularity of $G(x)$
3. $G(x_0) = \sum_{n=0}^{\infty} G_n x_0^n$
4. $H(x, G(x)) = 0$ if $|x| < |x_0|$
5. $\left. \frac{\partial H}{\partial y(x)} \right|_{(x_0, G(x_0))} = 0$

$$6. \left. \frac{\partial^2 H}{\partial y(x)^2} \right|_{(x_0, G(x_0))} \neq 0$$

Then

$$G(x) = G(x_0) + \sum_{k=1}^{\infty} a_k (x_0 - x)^{\frac{k}{2}}$$

and if $a_1 \neq 0$ then

$$G_n \rightarrow \sqrt{\frac{a_1^2 x_0}{4\pi}} x_0^{-n} n^{-\frac{3}{2}}$$

or if $a_1 = 0$ and $a_3 \neq 0$ then

$$G_n \rightarrow \sqrt{\frac{9a_3^2 x_0^3}{16\pi}} x_0^{-n} n^{-\frac{5}{2}}$$

1 Planted Trees

We start our branch node asymptotic analysis with Planted trees. Before we apply the theorem we must ensure that all 6 conditions are met. First will define the function $H_y(x, z)$ to be

$$H_y(x, z) = x^2 + xz + \frac{yz^2}{2} + \frac{yF_{y^2}(x^2)}{2} - z \quad (6)$$

If we recall the functional equation for $F_y(x)$:

$$F_y(x) = x^2 + xF_y(x) + \frac{y}{2}F_y^2(x) + \frac{y}{2}F_{y^2}(x^2) \quad (7)$$

Then clearly $z = F_y(x)$ is a solution to the equation $H = 0$ when $F_y(x)$ converges. So if we can show that $F_y(x)$ converges if $|x| \leq x_0(y)$ for some value $x_0(y)$ that is the radius of converge of $F_y(x)$ then we will have shown that conditions 1, 2, 3, and 4 hold. We will begin by showing that $x_0(y)$ exists for all y . There are three possible cases: $y < 1, y > 1, y = 1$. The $y = 1$ is trivial. We have shown that $F_1(x) = F(x)$ and we showed previously that $F(x)$ converges for all $x \leq x_0 = .4026975...$. The $y < 1$ is also quite simple. When $y < 1$ the $F_{nb}y^b < F_{nb}$ so it follows that

$$\sum_{b=0}^n F_{nb}y^b < \sum_{b=0}^n F_{nb}$$

so we can conclude that

$$F_n(y) < F_n \quad \text{for all } n \text{ if } y < 1 \quad (8)$$

So clearly $F_y(x)$ will converge for $x_0 = .4026975...$ So.

$$.4026975... \leq x_0(y) < 1 \quad \text{if } y \leq 1 \quad (9)$$

Thus $x_0(y)$ exists for $y \leq 1$ Finally, we must deal with the $y > 1$ case. First will briefly show that if $b \geq \frac{n}{2}$ then $F_{nb} = 0$. We will start by defining c to be the number of nodes with 2 branches and e to be the number of nodes with one branch (end nodes). Then clearly we may write for any tree.

$$b + c + e = n \quad (10)$$

we can also note that whenever we add another branch point we necessarily create another end point. Combining this observation with the fact that a tree with no branch points has two end points, we may write for all trees that.

$$b + 2 = e \quad (11)$$

we may combine Eq. 10 and Eq. 11 to get

$$2b = n - c - 2 \quad (12)$$

now we wish to maximize our branch point. To do this we can simply set $c = 0$ in Eq. 12 and then we get $2b = n - 2$ or more simply

$$b < \frac{n}{2} \quad (13)$$

This means there are no trees where the number of branch points is $\frac{n}{2}$ or higher. So we can conclude that if $b \geq \frac{n}{2}$ then $F_{nb} = 0$. now let us turn back to the case where $y > 1$ let us choose $x = \frac{x_0}{y}$ where $x_0 = .4026975$. Then

$$F_n(y)x^n = \left(\sum_{b=0}^n F_{nb}y^b \right) \left(\frac{x_0}{y} \right)^n \quad (14)$$

But since $F_{nb} = 0$ if $b \geq \frac{n}{2}$ we can write

$$F_n(y)x^n = \left(\sum_{b=0}^{n/2} F_{nb}y^b \right) \left(\frac{x_0}{y} \right)^n = \left(\sum_{b=0}^{n/2} F_{nb}y^{b-n} \right) x_0^n \quad (15)$$

Then since $b < \frac{n}{2} < n$ and $y > 1$, it follows that $y^{b-n} < 1$ so

$$\left(\sum_{b=0}^{n/2} F_{nb}y^{b-n} \right) x_0^n < F_n x_0^n \quad (16)$$

Then by the comparison test $F_y(\frac{x_0}{y})$ converges if $y > 1$. so we can conclude that

$$\frac{x_0}{y} \leq x_0(y) < 1 \quad \text{if } y > 1 \quad (17)$$

So we have finally shown that $x_0(y)$ exists for all y . This shows that $F_y(x)$ converges if $x < x_0(y)$. It remains to show that $F_y(x)$ converges at $x = x_0(y)$. To show this we will show that

$$\lim_{x \rightarrow x_0(y)^-} F_y(x) \text{ exists}$$

Since the power series $F_y(x)$ always has positive coefficients and positive powers of x , it is a monotonically increasing function so to show that this limit exists we must simply show that $F_y(x)$ is bounded above. It follows from the functional equation that

$$F_y(x) > \frac{y}{2} F_y^2(x)$$

Which then implies that

$$\frac{2}{y} > F_y(x) \quad (18)$$

thus $F_y(x)$ is bounded above so the limit exists and therefore $F_y(x_0(y))$ converges. Combining all of these results, we get that

$$F_y(x) \text{ converges if } |x| \leq x_0(y) \quad (19)$$

which shows that conditions 1, 2, 3, and 4 are all met.

Condition 5 is shown using the same proof by contradiction using the Implicit Function Theorem that we used for the non-branch-node-counting series. Condition 6 is shown by differentiating Eq 6 with respect to z twice to get

$$\frac{\partial^2 H}{\partial z^2} = y \quad (20)$$

If we think of y as the fugacity ($e^{\frac{\mu_b}{k_B T}}$) it is clear that no possible values of μ_b or T will result in a value of 0 for y so condition 6 holds.

Before we fully apply the theorem let us an expression for $F_y(x_0(y))$. We can differentiate Eq. 6 and then apply condition 5 to get

$$0 = x_0 + y F_y(x_0(y)) - 1 \quad (21)$$

which can be rearranged to get

$$F_y(x_0(y)) = \frac{1 - x_0(y)}{y} \quad (22)$$

Now we may apply Theorem 1 and expand $F_y(x)$ as:

$$F_y(x) = F_y(x_0(y)) + \sum_{k=1}^{\infty} a_k (x_0 - x)^{k/2} \quad (23)$$

Then if we differentiate this expansion we get:

$$F'_y(x) = - \sum_{k=1}^{\infty} \frac{ka_k}{2} (x_0 - x)^{k/2-1} \quad (24)$$

Then we may combine Eq. 23 and Eq. 24 to get:

$$F'_y(x)(F_y(x_0(y)) - F_y(x)) = \frac{a_1^2}{2} + \mathcal{O}(x_0 - x)$$

Then if we take the limit as $x \rightarrow x_0(y)$ we get that

$$\lim_{x \rightarrow x_0(y)} F'_y(x)(F_y(x_0(y)) - F_y(x)) = \frac{a_1^2}{2} \quad (25)$$

But we may also differentiate Eq. 7, plug in Eq. 22, and rearrange to get:

$$\lim_{x \rightarrow x_0(y)} F'_y(x)(F_y(x_0(y)) - F_y(x)) = \frac{2yx_0(y) + 1 - x_0(y) + x_0(y)y^2 F'_{y^2}(x_0^2(y))}{y^2} \quad (26)$$

Then we can combine Eq. 25 and Eq. 26 and solve for a_1 to get

$$a_1 = \frac{1}{y} \sqrt{2(1 + x_0(y)(y^2 F'_{y^2}(x_0^2(y)) + 2y - 1))} \quad (27)$$

So then by Theorem 1, we can write our asymptotic form as

$$F_n(y) \approx \sqrt{\frac{x_0(y) + x_0^2(y)(y^2 F'_{y^2}(x_0^2(y)) + 2y - 1)}{2\pi y^2}} x_0^{-n}(y) n^{-3/2} \quad (28)$$

There is still one problem. The method we used for finding the radius of convergence, taking the limit of the ration of the terms, takes 10,000 terms to get with in 3 decimal places of accuracy. Now that computing the coefficients involves a sum (see Eq. 4). so computing these coefficients to very high n becomes unreasonable. We need a way to find the radius of convergence of $F_y(x)$ using as few terms as possible. Let us plug in $x_0(y)$ for x in Eq. 6.

$$F_y(x_0(y)) = x_0(y)^2 + x_0(y)F_y(x_0(y)) + \frac{y}{2}F_y^2(x_0(y)) + \frac{y}{2}F_{y^2}(x_0^2(y))$$

And then we can substitute in Eq. 22 and rearrange to get the following equation:

$$F_{y^2}(x_0^2(y)) = \frac{1 + 2x_0(y) + (1 - 2y)x_0^2(y)}{y^2} \quad (29)$$

We can use Mathematica to numerically solve this equation for $x_0(y)$ and get more accurate answers by adding more terms on to the power series $F_{y^2}(x_0^2(y))$. This method only requires 10 terms in the power series to get 6 decimal places of accuracy. This huge jump in accuracy is due to the fact $x_0^2(y)$ is well inside the radius of convergence so we can get a very accurate estimate of $(F_{y^2}(x_0^2(y)))$ with just a few terms and by substituting Eq. 22 in we get an exact value for $F_y(x_0(y))$. All of this results in a quick and easy method for finding $x_0(y)$ for each y .

2 General Trees

We now turn our attention to general trees. Again, we will use the notations

$$T_y(x) \equiv T(x, y) \quad (30)$$

$$T_n(y) \equiv \sum_{b=0}^{\infty} T_{nb} y^b \quad (31)$$

to highlight the fact we will be treating the series as a single variable power series where the coefficients depend on y . We may write:

$$T_y(x) = \sum_{n=0}^{\infty} T_n(y) x^n \quad (32)$$

We must first confirm that $T_y(x)$ meets all 6 nessessary conditions so we may apply Theorem 1. Let us first write $H(x, z)$ as

$$H(x, z) = R_y(x) - \frac{F_y^2(x)}{2x^2} + \frac{F_{y^2}(x^2)}{2x^2} - z \quad (33)$$

So clearly $z = T_y(x)$ is a solution to $H(x, z) = 0$ whenever $T_y(x)$ converges. Then conditions 1, 2, 3, and 4 will hold if we can show that for some $x_T(y)$, $T_y(x)$ converges for all $x \leq x_T(y)$.

The functional equation for $T_y(x)$ is

$$T_y(x) = R_y(x) - \frac{F_y^2(x)}{2x^2} + \frac{F_{y^2}(x^2)}{2x^2} \quad (34)$$

Where $R_y(x)$ is

$$R_y(x) = x + F_y(x) + \frac{F_y(x)}{xy} - \frac{x}{y} - \frac{F_y(x)}{y} + \frac{yF_y^3(x)}{6x^2} + \frac{yF_{y^2}(x^2)F_y(x)}{2x^2} + \frac{yF_{y^3}(x^3)}{3x^2} \quad (35)$$

And then we may combine the two to get

$$T_y(x) = x + F_y(x) + \frac{F_y(x)}{xy} - \frac{x}{y} - \frac{F_y(x)}{y} + \frac{yF_y^3(x)}{6x^2} + \frac{yF_{y^2}(x^2)F_y(x)}{2x^2} + \frac{yF_{y^3}(x^3)}{3x^2} - \frac{F_y^2(x)}{2x^2} + \frac{F_{y^2}(x^2)}{2x^2} \quad (36)$$

So we can think of $T_y(x)$ as a function of $x, F_y(x), F_{y^2}(x^2)$, and $F_{y^3}(x^3)$. This means that $T_y(x)$ will converge whenever $F_y(x), F_{y^2}(x^2)$, and $F_{y^3}(x^3)$ converge. $F_y(x), F_{y^2}(x^2)$, and $F_{y^3}(x^3)$ have a radii of convergence of $x_0(y), \sqrt{x_0(y^2)}$, and $\sqrt[3]{x_0(y^3)}$ respectively. So we observe that

$$T_y(x) \text{ converges if } x \leq \min\{x_0(y), \sqrt{x_0(y^2)}, \sqrt[3]{x_0(y^3)}\}$$

We will show that $x_0(y) = \min\{x_0(y), \sqrt{x_0(y^2)}, \sqrt[3]{x_0(y^3)}\}$. It follows easily fom the triangle inequality that

$$\left(\sum_{b=0}^n F_{nb} y^b \right)^2 \geq \sum_{b=0}^n F_{nb} y^{2b}$$

Which we can write more compactly as

$$F_n^2(y) \geq F_n(y^2) \quad \text{For all } n \quad (37)$$

Then we consider the following two power series

$$P_1(x) = \sum_{n=0}^{\infty} F_n^2(y) x^n \quad (38)$$

$$P_2(x) = \sum_{n=0}^{\infty} F_n(y^2) x^n \quad (39)$$

Let thier radii of convergence be r_1 and r_2 respectively. Then because of Eq. 37 we may deduce that $r_1 \leq r_2$. but we may also write r_1 and r_2 as

$$r_1 = \lim_{n \rightarrow \infty} \left(\frac{F_n^2(y)}{F_{n+1}^2(y)} \right)^2 = x_0^2(y)$$

$$r_2 = \lim_{n \rightarrow \infty} \frac{F_n(y^2)}{F_{n+1}(y^2)} = x_0(y^2)$$

So we may conclude that $x_0^2(y) \leq x_0(y^2)$ or

$$x_0(y) \leq \sqrt{x_0(y^2)} \quad (40)$$

In a very similar way we can show

$$x_0(y) \leq \sqrt[3]{x_0(y^3)}$$

so we can conclude that

$$T_y(x) \text{ converges if } x \leq x_0(y)$$

and thus conditions 1, 2, 3, and 4 hold. Condition 5 holds Via the Inverse Function Theorem just as it did before and condition 6 holds as well. Then we may apply Theorem 1 and expand $T_y(x)$ as

$$T_y(x) = T_y(x_0(y)) + \sum_{k=1}^{\infty} b_k(x_0(y) - x)^{k/2} \quad (41)$$

Now we must find the value of b_1 . From differentiating the expansion we find

$$T'_y(x) = -\frac{b_1}{2}(x_0(y) - x)^{-1/2} - b_2 - \frac{3b_3}{2}(x_0(y) - x)^{1/2} + \dots \quad (42)$$

So as x gets close to $x_0(y)$ all terms except the first two go to zero while the first term blows up. So close to $x_0(y)$ the first term dominates the behavior of the function.

$$\lim_{x \rightarrow x_0(y)} T'_y(x) = -\frac{b_1}{2}(x_0(y) - x)^{-1/2} \quad (43)$$

But, we may also differentiate Eq. 34 to get

$$\begin{aligned} T'_y(x) = & 1 + F'_y(x) + \frac{F'_y(x)}{xy} - \frac{F_y(x)}{x^2y} - \frac{1}{y} - \frac{F'_y(x)}{y} + \frac{yF_y^2(x)F'_y(x)}{2x^2} - \frac{yF_y^3(x)}{3x^3} + \frac{yF_{y^2}(x^2)F'_y(x)}{2x^2} + \frac{yF'_{y^2}(x^2)F_y(x)}{x} \\ & - \frac{yF_{y^2}(x^2)F_y(x)}{x^3} + yF'_{y^3}(x^3) - \frac{2yF_{y^3}(x^3)}{3x^2} - \frac{yF_y(x)F'_y(x)}{x^2} + \frac{F_y^2(x)}{x^3} + \frac{F'_{y^2}(x^2)}{x} - \frac{F_{y^2}(x^2)}{x^3} \end{aligned} \quad (44)$$

Every term that does not have an $F'_y(x)$ converges as $x \rightarrow x_0(y)$ while every term that does blows up. So as x gets close to $x_0(y)$ the behavior of the $F'_y(x)$ terms dominate. So

$$\lim_{x \rightarrow x_0(y)} T'_y(x) = \lim_{x \rightarrow x_0(y)} F'_y(x) \left(1 + \frac{1}{xy} - \frac{1}{y} + \frac{1}{x^2} \left(\frac{yF_y^2(x)}{2} + \frac{yF_{y^2}(x^2)}{2} - F_y(x) \right) \right) \quad (45)$$

Then we may use Eq. 7, Eq.24, and Eq. 43 to get

$$b_1 = a_1 \left(\frac{1}{x_0(y)y} - \frac{1}{y} - \frac{F_y(x_0(y))}{x_0} \right)$$

Which simplifies using Eq. 22 to

$$b_1 = 0 \quad (46)$$

Since $b_1 = 0$ we must find the value of b_3 and use the second approximation to find our asymptotic formula. To do this we must take the second derivative of $T_y(x)$. However, it is useful to use a few tricks to remove all of the $F'_y(x)$ terms from Eq. 44 (we are able to do this because $T'_y(x)$ converges at $x_0(y)$). Then when we differentiate $T'_y(x)$ we wont have any $F''_y(x)$ terms so the only divergent terms will again be those with $F'_y(x)$. Then when we take the limit as $x \rightarrow x_0(y)$ we will not have a weird mix of $F'_y(x)$ and $F''_y(x)$ terms contributing to the behavior. So we recall that

$$T'_y(x) = F'_y(x) \left(\frac{1}{xy} - \frac{1}{y} - \frac{F_y(x)}{x} \right) + \dots$$

which can be simplified to

$$T'_y(x) = \frac{F'_y(x)}{xy} (1 - x - yF_y(x)) + \dots \quad (47)$$

Then, by differentiating Eq 7. we can show that

$$F'_y(x)(1 - x - yF_y(x)) = 2x + F_y(x) + xyF_{y^2}(x^2) \quad (48)$$

Substituting this into Eq.47 and adding the rest of the terms in we get

$$\begin{aligned} T'_y(x) = & \frac{2}{y} + \frac{F_y(x)}{xy} + F'_{y^2}(x^2) + 1 - \frac{F_y(x)}{x^2y} - \frac{1}{y} - \frac{yF_y^3(x)}{3x^3} + \frac{yF'_{y^2}(x^2)F_y(x)}{x} \\ & - \frac{yF_{y^2}(x^2)F_y(x)}{x^3} + yF'_{y^3}(x^3) - \frac{2yF_{y^3}(x^3)}{3x^2} + \frac{F_y^2(x)}{x^3} + \frac{F'_{y^2}(x^2)}{x} - \frac{F_{y^2}(x^2)}{x^3} \end{aligned} \quad (49)$$

Now we will take the second derivative of $T_y(x)$. Eventually, we will take the limit as $x \rightarrow x_0(y)$. Then, divergent terms such as $T_y''(x)$ and $F_y'(x)$ will dominate. So when taking the derivative we only care about the terms with $F_y'(x)$ so only those terms will be displayed in the interest in keeping the equation relatively compact. We get

$$T_y''(x) = F_y'(x) \left(\frac{1}{xy} - \frac{1}{x^2y} + \frac{yF_{y^2}'(x^2)}{x} - \frac{yF_y^2(x)}{x^3} - \frac{yF_{y^2}(x^2)}{x^3} + \frac{2F_y(x)}{x^3} \right) + \dots \quad (50)$$

Then we may take the limit as $x \rightarrow x_0(y)$ and use Eq. 7 to simplify

$$\lim_{x \rightarrow x_0(y)} T_y''(x) = \lim_{x \rightarrow x_0(y)} F_y'(x) \left(\frac{1}{x_0(y)y} - \frac{1}{x_0^2(y)y} + \frac{yF_{y^2}'(x_0^2(y))}{x} + \frac{1}{x^3} \left(2x_0^2(y) + 2x_0(y)F_y(x_0(y)) \right) \right) \quad (51)$$

which can be simplified further using Eq. 22 to get

$$\lim_{x \rightarrow x_0(y)} T_y''(x) = \lim_{x \rightarrow x_0(y)} F_y'(x) \left(\frac{2yx_0(y) + x_0(y)y^2F_{y^2}'(x_0^2(y)) + 1 - x_0(y)}{yx_0^2(y)} \right) \quad (52)$$

And then we can differentiate Eq. 42 (remembering that $b_1 = 0$) and use Eq. 24 and Eq. 27 to get

$$\frac{3b_3}{4} = \left(\frac{a_1}{2} \right) \left(\frac{ya_1^2}{2x_0^2(y)} \right) \quad (53)$$

which then gives us

$$b_3 = \frac{ya_1^3}{3x_0^2(y)} \quad (54)$$

So we get the following approximation for $T_n(y)$ using Theorem 1

$$T_n(y) \approx \frac{ya_1^3}{4\sqrt{\pi x_0(y)}} x_0^{-n}(y) n^{-5/2} \quad \text{where } a_1 = \frac{1}{y} \sqrt{2(1 + x_0(y)(y^2F_{y^2}'(x_0^2(y)) + 2y - 1))} \quad (55)$$

Or, if we let $\alpha = \frac{a_1}{2} \sqrt{\frac{x_0(y)}{\pi}}$ which was our coefficient from the asymptotic expansion of planted trees we can equivalently write

$$T_n(y) \approx \frac{2\pi y \alpha^3}{x_0^2(y)} x_0^{-n}(y) n^{-5/2} \quad (56)$$

3 Grand Partition Function

We have already stated that the coefficients we just approximated $T_n(y)$ generalize our former approximation for T_n as a partition function for an annealed branched polymer of n nodes into both a a partition function for n nodes into a grand partition function on branch points by associating a fugocity, y , with the creation/destruction of a branch node. We have just completed an approximation for this mixed partition function in the form of Eq. 56. But we may go even further. Let us consider using Eq. 56 to write an approximate form of $T_y(x)$.

$$T_y(x) = \sum_{n=0}^{\infty} \frac{2\pi y \alpha^3}{x_0^2(y)} n^{-5/2} \left(\frac{x}{x_0(y)} \right)^n \quad (57)$$

We can imagine that the eginnumber of nodes on a polymer is not fixed. physically this can be thought of as polymers splitting or combining to form smaller or larger polymers (this does actually happen). Then we may associate another chemical potential, μ_n , with the splitting or recombining of the polymers. Then using the same logic we used for the branch nodes we can think of x as the fugocity of splitting/recombination

$$x = e^{\frac{\mu_n}{k_B T}} \quad (58)$$

Then $T_y(x)$ becomes a grand partition function for both branch nodes and total nodes.

$$\Xi(\mu_b, \mu_n) = T_y(x) = \sum_{n=0}^{\infty} \frac{2\pi y \alpha^3}{x_0^2(y)} n^{-5/2} \left(\frac{x}{x_0(y)} \right)^n \quad \text{where } x = e^{\beta \mu_n}, y = e^{\beta \mu_b}, \text{ and } \beta = \frac{1}{k_B T} \quad (59)$$

4 Free Energy and Thermal Average Branch Points

Now that we have the partition function we can use it to get some results. Our partition function may be written as

$$Z(\mu, n, T) = e^{-\beta E_0} \frac{y a_1^3}{4\sqrt{\pi x_0(y)}} x_0^{-n}(y) n^{-5/2} \quad \text{where } y = e^{\beta\mu} \quad (60)$$

The Grand Potential, a type of free energy can be computed from the partition function using the relation

$$\Phi(\mu, n, T) = \frac{-\ln(Z)}{\beta} \quad (61)$$

Then applying Eq. 61 to Eq. 60 we get

$$\Phi(\mu, n, T) = E_0 - \mu + k_B T \left(\left(n + \frac{1}{2}\right) \ln(x_0(y)) + \frac{5}{2} \ln(n) + \ln(4\sqrt{\pi}) - 3 \ln(a_1(y)) \right) \quad (62)$$

This is the free energy associated with our branch counting model of the polymer. It is a Grand Potential in terms of branch points and a Helmholtz Free Energy in terms of n making it a mixed potential. From this mixed potential we can get all sorts of useful things. One such thing is a Thermal average of the branch points, $\langle b \rangle$ which can be found by differentiating the mixed potential with respect to the chemical potential of a branch point.

$$\langle b \rangle = -\frac{\partial \Phi}{\partial \mu} \quad (63)$$

By applying Eq. 63 to Eq. 62 we can get an expression for the average branch points. We get

$$\langle b \rangle = 1 + \frac{1}{\beta} \left(3 \frac{\partial}{\partial \mu} \ln(a_1(y)) - \left(n + \frac{1}{2}\right) \frac{\partial}{\partial \mu} \ln(x_0(y)) \right) \quad (64)$$

which can be simplified using the chain rule as:

$$\langle b \rangle = 1 + \frac{1}{\beta} \left(\frac{3}{a_1(y)} \frac{\partial a_1(y)}{\partial y} \frac{\partial y}{\partial \mu} - \frac{\left(n + \frac{1}{2}\right)}{x_0(y)} \frac{\partial x_0(y)}{\partial y} \frac{\partial y}{\partial \mu} \right) \quad (65)$$

Then we recall that $y = e^{\beta\mu}$ so

$$\frac{\partial y}{\partial \mu} = \beta y$$

which allows us to simplify Eq. 65 to

$$\langle b \rangle = 1 + \frac{3y}{a_1(y)} \frac{\partial a_1(y)}{\partial y} - \frac{y\left(n + \frac{1}{2}\right)}{x_0(y)} \frac{\partial x_0(y)}{\partial y} \quad (66)$$

We can easily compute $\frac{\partial x_0(y)}{\partial y}$ numerically using Mathematica. All that remains is to calculate $\frac{\partial a_1(y)}{\partial y}$. First let us realize that $a_1(y)$ is most easily expressed as a function of y and $x_0(y)$. Then $\frac{\partial a_1(y)}{\partial y}$ may be calculated using the chain rule as:

$$\frac{\partial a_1(y, x_0)}{\partial y} = \frac{\partial x_0}{\partial y} \left(\frac{\partial a_1(y, x_0)}{\partial x_0} \right)_y + \left(\frac{\partial a_1(y, x_0)}{\partial y} \right)_{x_0}$$

For the time being, we will write x_0 rather than $x_0(y)$ because we will be treating it as a variable rather than a function. then let us define the differential operator

$$\partial_y \equiv \frac{\partial x_0}{\partial y} \left(\frac{\partial}{\partial x_0} \right)_y + \left(\frac{\partial}{\partial y} \right)_{x_0} \quad (67)$$

Now let us rewrite Eq. 27 as

$$\frac{a_1^2}{2x_0} - \frac{1}{x_0 y^2} - \frac{2}{y} + \frac{1}{y^2} = F'_{y^2}(x_0^2) \quad (68)$$

Then if we apply ∂_y to both sides we get

$$\frac{a_1}{x_0} \partial_y a_1 - \frac{a_1^2}{2x_0^2} \frac{\partial x_0}{\partial y} + \frac{1}{y^2 x_0^2} \frac{\partial x_0}{\partial y} + \frac{2}{x_0 y^3} + \frac{2}{y^2} - \frac{2}{y^3} = \partial_y F'_{y^2}(x_0^2) \quad (69)$$

Then solving for $\partial_y a_1$ we get

$$\partial_y a_1 = \frac{\partial x_0}{\partial y} \left(\frac{a_1}{2x_0} - \frac{1}{y^2 x_0 a_1} \right) + \frac{2}{a_1 y^3} ((1-y)x_0 - 1) + \frac{x_0}{a_1} \partial_y F'_{y^2}(x_0^2) \quad (70)$$

But then the question becomes what is $\partial_y F'_{y^2}(x_0^2)$. If we differentiate Eq 1 and substitute in x_0^2 for x and y^2 for y , we get that

$$F'_{y^2}(x_0^2) = \sum_{n=0}^{\infty} \sum_{b=0}^{\infty} F_{nb} y^{2b} n x_0^{2n-2} \quad (71)$$

Then after applying ∂_y to Eq. 71 we get

$$\partial_y F'_{y^2}(x_0^2) = \frac{\partial x_0}{\partial y} \sum_{n=0}^{\infty} \sum_{b=0}^{\infty} F_{nb} y^{2b} (2n^2 - 2n) x_0^{2n-3} + \sum_{n=0}^{\infty} \sum_{b=0}^{\infty} F_{nb} 2b y^{2b-1} n x_0^{2n-2} \quad (72)$$

which simplifies to

$$\partial_y F'_{y^2}(x_0^2) = \sum_{n=0}^{\infty} \sum_{b=0}^{\infty} F_{nb} y^{2b} \left(\frac{2bn}{y} + \frac{\partial x_0}{\partial y} \frac{2n^2 - 2n}{x_0} \right) x_0^{2n-2} \quad (73)$$

Then we may write that

$$\partial_y F'_{y^2}(x_0^2) = \Gamma(y) \quad \text{where } \Gamma(y) \equiv \sum_{n=0}^{\infty} \gamma_n(y) x_0^{2n-2} \text{ and } \gamma_n(y) \equiv \sum_{b=0}^{\infty} F_{nb} y^{2b} \left(\frac{2bn}{y} + \frac{\partial x_0}{\partial y} \frac{2n^2 - 2n}{x_0} \right) \quad (74)$$

Then using Eq. 74 we may rewrite Eq. 70 and plug it into Eq. 66 to get

$$\langle b \rangle = 1 + \frac{3y}{a_1} \left(\frac{\partial x_0}{\partial y} \left(\frac{a_1}{2x_0} - \frac{1}{y^2 x_0 a_1} \right) + \frac{2}{a_1 y^3} ((1-y)x_0 - 1) + \frac{x_0}{a_1} \Gamma(y) \right) - \frac{y(n + \frac{1}{2})}{x_0(y)} \frac{\partial x_0(y)}{\partial y} \quad (75)$$

which simplifies to

$$\langle b \rangle = 1 - \frac{\partial x_0(y)}{\partial y} \frac{3}{y x_0 a_1^2} + \frac{6}{a_1^2 y^2} ((1-y)x_0 - 1) + \frac{3x_0 y}{a_1^2} \Gamma(y) - \frac{y(n-1)}{x_0(y)} \frac{\partial x_0(y)}{\partial y} \quad (76)$$

Then notice if we define

$$A(\mu) \equiv -\frac{y}{x_0(y)} \frac{\partial x_0(y)}{\partial y} \quad (77)$$

and

$$B(\mu) \equiv 1 - A(\mu) - \frac{3}{y x_0(y) a_1^2(y)} \frac{\partial x_0(y)}{\partial y} + \frac{6}{a_1^2(y) y^2} ((1-y)x_0(y) - 1) + \frac{3x_0(y)y}{a_1^2(y)} \Gamma(y) \quad (78)$$

We can rewrite Eq. 76 as

$$\langle b \rangle = A(\mu)n + B(\mu) \quad (79)$$

which reduces the expression for $\langle b \rangle$ to a linear equation in terms of n where the coefficient depends on μ . Additionally, it turns out that $B(\mu)$ is always on the order of single digits so since we are already dealing with large n , we can ignore the $B(\mu)$ term. So then Eq. 76 may be written as

$$\frac{\langle b \rangle}{n} = A(\mu) \quad (80)$$

This shows that, for a fixed value of μ , the ratio of average branch points to total points is roughly a constant!