# DETAILED ASYMPTOTIC ANALYSIS: THE $\pi$-SHAPES CASE 

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#### Abstract

We present a detailed analysis for asymptotical number of case of $\pi$-shapes, similar to that of the RNA secondary structures.


## 1. Introduction

In this section, we give a self-contained justification of the application of the Odlyzko-Flajolet theorem (2) to obtain the asymptotic number of $\pi$-shapes compatible with secondary structures on $n$. Recall that if $S(z)=$ $\sum_{n=0}^{\infty} S_{n} z^{n}$ is the generating function for $\pi$-shapes compatible with secondary structures on $n$, it is given by

$$
S(z)=\frac{1-z^{5}-\sqrt{1-2 z^{5}-4 z^{7}+z^{10}}}{2(1-z) z^{2}}
$$

We begin by discussing why the square root function is not analytic, and why the exponential growth rate of $S_{n}$ is determined by the dominant singularity.

## 2. Why the square root is not analytic

The definition of a function $f$ being analytic at a point $z_{0}$ is that the complex derivative of $f$ is defined at $z_{0}$. Note that while the function $\sqrt{z}$ is defined at $\mathrm{z}=0$, it is not analytic at $\mathrm{z}=0$. The derivative of $\sqrt{z}=z^{1 / 2}$ is $\frac{1}{2} z^{-1 / 2}$. As is suggested by this, the derivative does not exist at zero. One can directly find this by showing that the Cauchy-Riemann equations are not satisfied (if they are, the complex derivative exists), but it's ugly. One can also use the Cauchy integral theorem. In any case, $\sqrt{z}$ is analytic everywhere except 0 .

## 3. BACK TO TASK, EXPONENTIAL GROWTH FACTOR

Similarly the function $\sqrt{1-2 z^{5}-4 z^{7}+z^{10}}$ is not analytic exactly at the zeros of the polynomial $1-2 z^{5}-4 z^{7}+z^{10}$. And the function,

$$
S=\frac{1-z^{5}-\sqrt{1-2 z^{5}-4 z^{7}+z^{10}}}{2(1-z) z^{2}}
$$

[^0]is analytic everywhere except the zeros of the polynomial inside the square root, and possibly where the denominator equals 0 .

It is known from introductory complex analysis that a power series converges in a circular region about the point of expansion out to the nearest non-analytic point, or singularity. In addition, if the singularity is not trivial ${ }^{1}$ the power series always diverges outside of this circle. (See the chapter on power series in Churchill's Complex Variables and Applications (1) for a good and quick introduction.)

This fact gives an immediate answer for the exponential growth of the power series terms of a given function. In the case of generating series, we are expanding about the point $z=0$. For a generating series with positive coefficients, it can be shown, using Pringsheim's theorem (3), that the singularity closest to the origin always occurs on the positive real axis at some value $\rho$. Then, we know that the power series converges for the circular region $|z|<\rho$, and so the exponential growth of the terms $f_{n}$ cannot be greater than $(1 / \rho)^{n}$. Otherwise, if the terms grow faster than this, it is clear that the series

$$
f(z)=\sum_{n=0}^{\infty} f_{n} z^{n}
$$

cannot converge near $z=\rho$ as the terms aren't going to zero. Similarly, since the power series diverges for any $z$ such that $|z|>\rho$, the exponential growth rate of the terms cannot be less than $(1 / \rho)^{n}$. Otherwise it is straightforward to show the series will converge for real $z>\rho$. Thus we immediately get that for generating functions the exponential rate of growth of terms is exactly $(1 / \rho)$.

This singularity closest to the origin is called the dominant singularity. For our function S , the dominant singularity is at $\rho \approx 0.756328$, one of the roots of the polynomial $1-2 z^{5}-4 z^{7}+z^{10}$, which is inside the square root in $S(z)$. And we get immediately that for large $n, S$ scales as

$$
S_{n} \approx(1 / \rho)^{n} \approx(1 / 0.756328)^{n} \approx(1.32218)^{n}
$$

So, the above gives the exponential growth. In many cases, this is all that is desired. However, we still could be off by non-exponential growth factors. Thus, for example, if $\rho=1$, all we know is that there is no exponential growth or decay. Within these bounds, anything, for example polynomial growth, is possible.

[^1]
## 4. Finer asymptotics

To get the asymptotics more exactly is not hard either, that is, using the results from the paper by Flajolet and Odlyzko (2).

To use these results, we have to verify that the generating series is analytic in the region $\Delta$ shown in figure 1 , except at the point $\rho$, thus analytic in $\Delta \backslash \rho$, where for the shape $\triangle$ we can choose any $\varepsilon$ and $0<\phi<\pi / 2$. The region $\Delta$ is the solid circle about the origin with radius $\rho+\varepsilon$, with a symmetric wedge cut out of it, centered about the real axis, to the point $\rho$.

Since our singularities are isolated (this will always be true if you have only finitely many singularities), and our dominant singularity is unique, (that is, we do not have more than one singularity the same minimal distance from the origin) we can choose $\varepsilon$ to make our function analytic in $\Delta \backslash \rho$. Simply note that $\triangle$ is a subset of the solid circle of radius $\rho+\varepsilon$ about the origin. Thus, if all of our singularities have larger magnitude than $\rho$, they will have larger magnitude than $\rho+\varepsilon$ for some $\varepsilon$, and will not be in $\triangle$.

Note that this method can be applied in any case in which the singularities are isolated and the dominant singularity is unique. There are usually ways to work around cases where the dominant singularity is not unique.


Figure 1. The shaded region $\triangle$ where, except at $z=\rho$, the generating function $S(z)$ must be analytic

First some setup. We have our function

$$
S=\frac{1-z^{5}-\sqrt{1-2 z^{5}-4 z^{7}+z^{10}}}{2(1-z) z^{2}}
$$

Call the polynomial under the square root $P(z)$. Since $z=\rho$ is a root of $P(z)$ we can pull out the factor $\sqrt{1-z / \rho}$ (using Mathematica or Maple) to get

$$
\sqrt{P(z)}=\sqrt{1-z / \rho} \sqrt{P_{2}(z)}
$$

where now $\sqrt{P_{2}(z)}$ will be analytic for all $z$ such that $|z|<\rho+\varepsilon$ for some $\varepsilon$, so that for where we're interested in, $\sqrt{P_{2}(z)}$ is always analytic.

Split $S$ into 2 parts:

$$
\begin{aligned}
S(z) & =\frac{1-z^{5}}{2(1-z) z^{2}}-\frac{\sqrt{1-2 z^{5}-4 z^{7}+z^{10}}}{2(1-z) z^{2}} \\
g(z) & =\frac{1-z^{5}}{2(1-z) z^{2}} \\
h(z) & =-\frac{\sqrt{1-z / \rho} \sqrt{P_{2}(z)}}{2(1-z) z^{2}} \\
S(z) & =g(z)+h(z)
\end{aligned}
$$

If we didn't worry about being rigorous, we can quick pull out the asymptotics. If you don't care about being rigorous, you can skip the next section.

## 5. A detailed analysis

To apply the results of the paper by Flajolet and Odlyzko(2), we will need to rescale the relevant part of the function so that the dominant singularity is at 1 instead of at $\rho$.

Let

$$
\begin{aligned}
& G(z)=z^{2} g(z)=\frac{1-z^{5}}{2(1-z)} \\
& H(z)=z^{2} h(z)=-\frac{\sqrt{1-z / \rho} \sqrt{P_{2}(z)}}{2(1-z)}
\end{aligned}
$$

That way, $G(z)$ and $H(z)$ are both defined, and analytic, at 0 and we can talk about their power series expansion about 0 . Recall that Cauchy's formula is

$$
f_{n}=\left[z^{n}\right] f(z)=\frac{1}{2 \pi i} \oint_{O^{+}} \frac{f(z)}{z^{n+1}} d z,
$$

where $O^{+}$is any positively oriented contour in $\triangle$ (in an analytic region) that encloses the origin. In their proof, they're going to use a special contour, we don't have to worry about that.

Then,

$$
\begin{aligned}
S_{n} & =\frac{1}{2 \pi i} \oint \frac{S(z)}{z^{n+1}} d z \\
& =\frac{1}{2 \pi i} \oint \frac{g(z)}{z^{n+1}} d z+\oint \frac{h(z)}{z^{n+1}} d z \\
& =\frac{1}{2 \pi i} \oint \frac{G(z)}{z^{n+3}} d z+\oint \frac{H(z)}{z^{n+3}} d z \\
S_{n} & =G_{n+2}+H_{n+2}
\end{aligned}
$$

We figure out the asymptotics of $G$ and $H$.

$$
\begin{aligned}
G(z) & =\frac{1-z^{5}}{2(1-z)} \\
& =\frac{1}{2}\left(1+z+z^{2}+z^{3}+z^{4}\right)
\end{aligned}
$$

Thus $G_{n}$ is 0 for any large $n$. Note that even if this is not the case, more generally we know that $G(z)$ will grow exponentially like $1 /\left|\rho^{\prime}\right|$, where $\rho^{\prime}$ is the first place that the function $G(z)$ is not analytic (may be complex). Since $\left|\rho^{\prime}\right|>\rho$, this exponential growth rate will be slower than the growth rate of $H(z)$, so we can ignore it.

For $H(z)$, rescale so that the singularity occurs at $w=1$ instead of $z=\rho$. To do this, simply substitute $z=\rho w$. We get

$$
H(w)=-\frac{\sqrt{1-w} \sqrt{P_{2}(\rho w)}}{2(1-\rho w)}
$$



Figure 2. The shaded region $\triangle$ where, except at $w=1$, the generating function $H(w)$ must be analytic

The function $H(w)$ has a singularity at $w=1$, and is analytic in the required region, $\triangle \backslash 1$, where the rescaled region $\triangle$ is shown in figure 2 . Note that external singularities that remain will scale to still be outside of the region $\triangle$. We now apply the following theorem (stated as Corollary 2, part (i) of (2) on page 224) which states

Theorem. Assume that $\mathrm{f}(\mathrm{z})$ is analytic in $\triangle \backslash 1$, and that as $z \rightarrow 1$ in $\triangle$,

$$
f(z) \sim K(1-z)^{\alpha}
$$

Then, as $n \rightarrow \infty$, if $\alpha \notin 0,1,2, \ldots$,

$$
f_{n} \sim \frac{K}{\Gamma-\alpha} n^{-\alpha-1} .
$$

We take $\alpha=+1 / 2$. Note that

$$
f(z) \sim g(z)
$$

as $z \rightarrow z_{0}$ means

$$
\lim _{z \rightarrow z_{0}} \frac{f(z)}{g(z)}=1
$$

For our $H(w)$, we find

$$
\frac{H(w)}{(1-w)^{1 / 2}}=-\frac{\sqrt{P_{2}(\rho w)}}{2(1-\rho w)}
$$

so that

$$
\begin{aligned}
\lim _{w \rightarrow 1} \frac{H(w)}{(1-w)^{1 / 2}} & =-\frac{\sqrt{P_{2}(\rho)}}{2(1-\rho)}=K^{\prime} \\
\lim _{w \rightarrow 1} \frac{H(w)}{K^{\prime}(1-w)^{1 / 2}} & =1
\end{aligned}
$$

This can be rewritten

$$
H(w) \sim K^{\prime}(1-w)^{1 / 2}
$$

By the above theorem, we get

$$
\left[w^{n}\right] H(w) \sim \frac{K^{\prime}}{\Gamma(-1 / 2)} n^{-3 / 2}
$$

Now we scale back. Note that

$$
H(w)=\sum H_{n}^{w} w^{n}
$$

where in the term $H_{n}^{w}=\left[w^{n}\right] H(w)$, the superscript $w$ reminds us that these are the coefficients when we expand the function in terms of the variable $w$.

$$
\begin{aligned}
H(w) & =\sum H_{n}^{w} w^{n} \\
& =\sum H_{n}^{w} \frac{z^{n}}{\rho^{n}} \\
& =\sum \frac{H_{n}^{w}}{\rho^{n}} z^{n}
\end{aligned}
$$

Therefore, the $H_{n}=\left[z^{n}\right] H(z)$, the power series coefficients of $H$ in terms of $z$, are given by,

$$
H_{n}=\frac{H_{n}^{w}}{\rho^{n}}
$$

so that

$$
\begin{aligned}
H_{n} & \sim \frac{H_{n}^{w}}{\rho^{n}} \\
H_{n} & \sim \frac{K^{\prime}}{\Gamma(-1 / 2)}\left(\frac{1}{\rho}\right)^{n} n^{-3 / 2}
\end{aligned}
$$

Remember that for large $n$, the $G_{n}$ goes away so that

$$
S_{n}=H_{n+2} \sim \frac{K^{\prime}}{\Gamma(-1 / 2)}\left(\frac{1}{\rho}\right)^{n+2}(n+2)^{-3 / 2}
$$

And then note that

$$
\lim _{n \rightarrow \infty} \frac{(n+2)^{-3 / 2}}{n^{3 / 2}}=\lim _{n \rightarrow \infty}\left(\frac{n+2}{n}\right)^{3 / 2}=1
$$

so that

$$
(n+2)^{-3 / 2} \sim n^{-3 / 2}
$$

which means we can simplify to

$$
S_{n} \sim \frac{K^{\prime}}{\rho^{2} \Gamma(-1 / 2)}\left(\frac{1}{\rho}\right)^{n} n^{-3 / 2}
$$

or letting $K=K^{\prime} / \rho^{2}$,

$$
S_{n} \sim \frac{K}{\Gamma(-1 / 2)}\left(\frac{1}{\rho}\right)^{n} n^{-3 / 2}
$$

Plugging in values ( $\rho \approx 0.756328$ ) gives

$$
S_{n} \sim 1.84657(1.32218)^{n} n^{-3 / 2}
$$

These asymptotics have been verified by simulation of the corresponding recurrence relations to work.

## 6. The short way

Now that we can see how the theorem applies, how rescaling works, and that splitting the generating function into parts that are not analytic at 0 does not cause problems, we can see that if we start with

$$
\begin{aligned}
& g(z)=\frac{1-z^{5}}{2(1-z) z^{2}} \\
& h(z)=-\frac{\sqrt{1-z / \rho} \sqrt{P_{2}(z)}}{2(1-z) z^{2}} \\
& S(z)=g(z)+h(z)
\end{aligned}
$$

we can ignore $g(z)$ as it doesn't have the dominant singularity. Then we simply get K by taking out the $\sqrt{1-z / \rho}$ term and evaluating the rest of $h(z)$ at the dominant singularity $\rho$ to get

$$
K=-\frac{\sqrt{P_{2}(\rho)}}{2(1-\rho) \rho^{2}} \approx 1.84657
$$

Since the singularity is of the form $(1-z / \rho)^{1 / 2}$, we read off $\alpha=1 / 2$. We then take the general equation

$$
S_{n} \sim \frac{K}{\Gamma(-1 / 2)}\left(\frac{1}{\rho}\right)^{n} n^{-1-\alpha}
$$

and plug in our values to obtain our final answer.

$$
S_{n} \sim 1.84657(1.32218)^{n} n^{-3 / 2}
$$

## References

[1] R. V. Churchill. Complex Variables and Applications. McGraw-Hill, 1960.
[2] P. Flajolet and A. M. Odlyzko. Singularity analysis of generating functions. SIAM Journal of Discrete Mathematics, 3:216-240, 1990.
[3] A. I. Markushevich. Theory of Functions of a Complex Variable. Chelsea Publishing Company, 1977.

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[^1]:    ${ }^{1}$ All singularities we deal with will be what we call non-trivial. A function $f$ analytic inside a circle $C$ has a non-trivial singularity at $z_{0}$ on $C$ if either $f$ or its derivative of some order has no limit as $z$ tends to $z_{0}$ in $C$. An example of a trivial singularity is the singularity of the function $f(z)=e^{z}(z-1) /(z-1)$ at $z=1$.

