

14 Expression of Li Coefficients by Polygamma Functions

14.1 Sum of Reciprocals of Zeros and the Notation

Sum of Reciprocals of Zero Points

The sum of the reciprocals of the zeros of the Riemann Zeta function is generally written as

$$\lambda_1 = \sum_{\rho} \frac{1}{\rho} \quad (1.1)$$

This notation is conceptual and valid to this extent. However, this notation cannot describe the semi-multiple series of this reciprocal. For example, if we were to forcefully express λ_1^3 using this notation, it would look like

$$\left(\sum_{\rho} \frac{1}{\rho} \right)^3 = \sum_{\rho} \frac{1}{\rho^3} + 3 \left(\sum_{\rho} \frac{1}{\rho} \right) \sum_{\rho \rho} \frac{1}{\rho \rho} - 3 \sum_{\rho \rho \rho} \frac{1}{\rho \rho \rho} \quad (1.3)$$

where, in the double sum and triple sum, ρ is not duplicated.

However, this notation is inconvenient and practical calculations are impossible. Therefore, in this chapter we use the following notation:

(1) Complex number notation

$$\begin{aligned} & \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \\ & \sum_{r_1=1}^{\infty} \sum_{r_2=1+r_1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2}} \\ & \sum_{r_1=1}^{\infty} \sum_{r_2=1+r_1}^{\infty} \sum_{r_3=1+r_2}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3}} \\ & \sum_{r_1=1}^{\infty} \sum_{r_2=1+r_1}^{\infty} \sum_{r_3=1+r_2}^{\infty} \sum_{r_4=1+r_3}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3} \rho_{r_4}} \\ & \vdots \\ & \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \dots \sum_{r_n=r_{n-1}+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \dots \rho_{r_n}} \end{aligned}$$

(2) Real and imaginary parts notation

However, even with the notation (1), it is difficult to examine the real and imaginary parts of the zeros ρ_k in detail.

So, considering that the Riemann Zeta function has conjugate zeros, we replace ρ_k $k=1, 2, 3, \dots$ as follows.

$$\rho_1 = x_1 - iy_1, \rho_2 = x_1 + iy_1, \rho_3 = x_2 - iy_2, \rho_4 = x_2 + iy_2, \rho_5 = x_3 - iy_3, \rho_6 = x_3 + iy_3, \dots$$

Using this, the example (1) can be rewritten as follows.

$$\begin{aligned} \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} &= \sum_{r=1}^{\infty} \left(\frac{1}{x_r - iy_r} + \frac{1}{x_r + iy_r} \right) = \sum_{r=1}^{\infty} \frac{2x_r}{x_r^2 + y_r^2} \\ \sum_{r_1=1}^{\infty} \sum_{r_2=1+r_1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2}} &= \sum_{r=1}^{\infty} \sum_{s=1+r}^{\infty} \frac{2^2 x_r x_s}{(x_r^2 + y_r^2)(x_s^2 + y_s^2)} + \sum_{r=1}^{\infty} \frac{2^0}{x_r^2 + y_r^2} \\ \sum_{r_1=1}^{\infty} \sum_{r_2=1+r_1}^{\infty} \sum_{r_3=1+r_2}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3}} &= \sum_{r=1}^{\infty} \sum_{s=1+r}^{\infty} \sum_{t=1+s}^{\infty} \frac{2^3 x_r x_s x_t}{(x_r^2 + y_r^2)(x_s^2 + y_s^2)(x_t^2 + y_t^2)} \\ &+ \sum_{r=1}^{\infty} \sum_{s=1+r}^{\infty} \frac{2^1 (x_r + x_s)}{(x_r^2 + y_r^2)(x_s^2 + y_s^2)} \end{aligned}$$

$$\begin{aligned}
\sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \sum_{r_3=r_2+1}^{\infty} \sum_{r_4=r_3+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3} \rho_{r_4}} &= \sum_{r=1}^{\infty} \sum_{s=1+r}^{\infty} \sum_{t=1+s}^{\infty} \sum_{u=1+t}^{\infty} \frac{2^4 x_r x_s x_t x_u}{(x_r^2 + y_r^2)(x_s^2 + y_s^2)(x_t^2 + y_t^2)(x_u^2 + y_u^2)} \\
&+ \sum_{r=1}^{\infty} \sum_{s=1+r}^{\infty} \sum_{t=1+s}^{\infty} \frac{2^2 (x_r x_s + x_r x_t + x_s x_t)}{(x_r^2 + y_r^2)(x_s^2 + y_s^2)(x_t^2 + y_t^2)} \\
&+ \sum_{r=1}^{\infty} \sum_{s=1+r}^{\infty} \frac{2^0}{(x_r^2 + y_r^2)(x_s^2 + y_s^2)}
\end{aligned}$$

⋮

14.2 Li's Criterion and Li Coefficients

Li's criterion for the Riemann zeta function $\zeta(z)$ was as follows:

Li's Criterion

The Riemann hypothesis is equivalent to the inequality;

$$\lambda_n = \frac{1}{(n-1)!} \left. \frac{d^n}{dz^n} \left[(1-z)^{n-1} \log \xi(z) \right] \right|_{z=0} \geq 0 \quad \text{for } n=1, 2, 3, \dots$$

where,

$$\xi(z) = -z(1-z) \pi^{-\frac{z}{2}} \Gamma\left(\frac{z}{2}\right) \zeta(z)$$

When ρ is a non-trivial zero of the Riemann Zeta function $\zeta(z)$, it is known that the Li coefficient λ_n is equivalent to the following:

Li coefficient λ_n

$$\lambda_n = \sum_{\rho} \left(1 - \left(1 - \frac{1}{\rho} \right)^n \right)$$

where, the sum extends over all ρ .

The first few are expanded as follows:

$$\begin{aligned} \lambda_1 &= \sum_{\rho} \frac{1}{\rho} \\ \lambda_2 &= \sum_{\rho} \left(\frac{2}{\rho} - \frac{1}{\rho^2} \right) = 2 \sum_{\rho} \frac{1}{\rho} - \sum_{\rho} \frac{1}{\rho^2} \\ \lambda_3 &= \sum_{\rho} \left(\frac{3}{\rho} - \frac{3}{\rho^2} + \frac{1}{\rho^3} \right) = 3 \sum_{\rho} \frac{1}{\rho} - 3 \sum_{\rho} \frac{1}{\rho^2} + \sum_{\rho} \frac{1}{\rho^3} \\ \lambda_4 &= \sum_{\rho} \left(\frac{4}{\rho} - \frac{6}{\rho^2} + \frac{4}{\rho^3} - \frac{1}{\rho^4} \right) = 4 \sum_{\rho} \frac{1}{\rho} - 6 \sum_{\rho} \frac{1}{\rho^2} + 4 \sum_{\rho} \frac{1}{\rho^3} - \sum_{\rho} \frac{1}{\rho^4} \\ &\vdots \end{aligned}$$

Now, using the notation in the previous section, Li coefficients can be written as follows:

Lemma 14.2.1

If ρ_{r_1} $r_1 = 1, 2, 3, \dots$ are nontrivial zeros of the Riemann Zeta function $\zeta(z)$, the Li coefficients λ_n $n = 1, 2, 3, \dots$ are expressed as follows.

$$\begin{aligned} \lambda_1 &= \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \\ \lambda_2 &= 2 \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} - \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^2} \\ \lambda_3 &= 3 \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} - 3 \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^2} + \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^3} \\ \lambda_4 &= 4 \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} - 6 \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^2} + 4 \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^3} - \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^4} \end{aligned}$$

$$\begin{aligned} & \vdots \\ \lambda_n &= n \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} + \sum_{k=2}^n (-1)^{k-1} \binom{n}{k} \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^k} \end{aligned} \quad (2.1n)$$

Semi-multiple series representation of Li coefficients

Now, $\lambda_1, \lambda_2, \lambda_3, \dots$ can be expressed as the following semi-multiple series.

$$\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}}, \sum_{r_1=1}^{\infty} \sum_{r_2=1+r_1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2}}, \sum_{r_1=1}^{\infty} \sum_{r_2=1+r_1}^{\infty} \sum_{r_3=1+r_2}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3}}, \dots$$

To do so, we first need the following recurrence relation:

Lemma 14.2.2

When n is natural number s.t. $n \geq 2$, for a convergent infinite series, the following holds.

$$\begin{aligned} \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^n} &= \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \right)^n - 2 \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \right)^{n-2} H_2 \\ &\quad - \sum_{s=0}^{n-3} \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \right)^s \left\{ \sum_{t=2}^{n-s-1} (-1)^t \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^{n-s-t}} \right) H_t + (-1)^{n-s} (n-s) H_{n-s} \right\} \end{aligned} \quad (2.2n)$$

Where,

$$\begin{aligned} H_2 &= \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2}} \\ H_3 &= \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \sum_{r_3=r_2+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3}} \\ &\vdots \\ H_n &= \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \sum_{r_3=r_2+1}^{\infty} \dots \sum_{r_n=r_{n-1}+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3} \dots \rho_{r_n}} \end{aligned} \quad (2.Hn)$$

When $n \leq 2$, the 3 rd term of (2.2n) is ignored.

Proof

Theorem 5.2.2 on my site " **05 Power Series and Semi Multiple Series** " (Infinite Degree Equations) is as follows.

Theorem 5.2.2 (Reprint)

When n is natural number s.t. $n \geq 2$, for a convergent infinite series, the following holds.

$$\begin{aligned} \left(\sum_{r_1=1}^{\infty} a_{r_1} \right)^n &= \sum_{r_1=1}^{\infty} a_{r_1}^n + 2 \left(\sum_{r_1=1}^{\infty} a_{r_1} \right)^{n-2} H_2 \\ &\quad + \sum_{s=0}^{n-3} \left(\sum_{r_1=1}^{\infty} a_{r_1} \right)^s \left(\sum_{t=2}^{n-s-1} (-1)^t \left(\sum_{r_1=1}^{\infty} a_{r_1}^{n-s-t} \right) H_t + (-1)^{n-s} (n-s) H_{n-s} \right) \end{aligned}$$

Where,

$$\begin{aligned} H_2 &= \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} a_{r_1} a_{r_2} \\ H_3 &= \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \sum_{r_3=r_2+1}^{\infty} a_{r_1} a_{r_2} a_{r_3} \\ &\vdots \end{aligned}$$

$$H_n = \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \sum_{r_3=r_2+1}^{\infty} \cdots \sum_{r_n=r_{n-1}+1}^{\infty} a_{r_1} a_{r_2} a_{r_3} \cdots a_{r_n}$$

When $n \leq 2$, the 3 nd term is ignored.

Replacing a_{r_n} with $1/\rho_{r_n}$ in this theorem, we obtain Lemma 14.2.2 . Q.E.D.

On the other hand, the following relationship exists between the semi-multiple series in Lemma 14.2.2 and the coefficients of the Maclaurin series of $\xi(z)$.

Lemma 14.2.3

Let the function $\xi(z)$ and its Maclaurin series be

$$\xi(z) = -z(1-z) \pi^{-\frac{z}{2}} \Gamma\left(\frac{z}{2}\right) \zeta(z) = \sum_{r=0}^{\infty} A_r z^r$$

Then, the following equations hold for the zeros ρ_{r_1} $r_1 = 1, 2, 3, \dots$ of $\xi(z)$.

$$A_1 = - \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \tag{2.3_1}$$

$$A_2 = \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2}}$$

$$A_3 = - \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \sum_{r_3=r_2+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3}}$$

$$A_4 = \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \sum_{r_3=r_2+1}^{\infty} \sum_{r_4=r_3+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3} \rho_{r_4}}$$

⋮

$$A_n = (-1)^n \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \cdots \sum_{r_n=r_{n-1}+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \cdots \rho_{r_n}} \tag{2.3n}$$

Proof

$\xi(z)$ is completely factored by the zeros ρ_{r_1} $r_1 = 1, 2, 3, \dots$ as follows.

$$\xi(z) = \left(1 - \frac{z}{\rho_1}\right) \left(1 - \frac{z}{\rho_2}\right) \left(1 - \frac{z}{\rho_3}\right) \left(1 - \frac{z}{\rho_4}\right) \cdots$$

According to Formula 3.2.1 in my site " **03 Vieta's Formulas in Infinite-degree Equation** " (Infinite Degree Equations) , Vieta's formula also holds for infinite degree equations. Therefore, we obtain the desired expressions. Q.E.D.

And these values of A_n $n=1, 2, 3, 4, \dots$ are given by π and the higher derivatives of $\Gamma(z)$, $\zeta(z)$, which are the components of $\xi(z)$. That is, the coefficients A_r $r=1, 2, 3, \dots$ in Lemma 14.2.3 is given by Theorem 9.1.3 on my site " **09 Maclaurin Series of Completed Riemann Zeta** ". If we reprint this theorem in a slightly different form, it becomes:

Lemma 14.2.4

Let the completed Riemann zeta function $\xi(z)$ and the Maclaurin series be as follows.

$$\xi(z) = -z(1-z) \pi^{-\frac{z}{2}} \Gamma\left(\frac{z}{2}\right) \zeta(z) = \sum_{r=0}^{\infty} A_r z^r$$

Then, these coefficients A_r $r=0, 1, 2, 3, \dots$ are given by

$$A_r = \sum_{s=0}^r \sum_{t=0}^s \frac{\log^{r-s} \pi}{2^{r-s} (r-s)!} \frac{(-1)^{s-t} g_{s-t}(3/2)}{2^{s-t} (s-t)!} h_t$$

$$g_r\left(\frac{3}{2}\right) = \begin{cases} 1 & r = 0 \\ \sum_{k=1}^r B_{r,k}\left(\psi_0\left(\frac{3}{2}\right), \psi_1\left(\frac{3}{2}\right), \dots, \psi_{r-1}\left(\frac{3}{2}\right)\right) & r = 1, 2, 3, \dots \end{cases}$$

$$h_r = \begin{cases} 1 & r = 0 \\ -\frac{\gamma_{r-1}}{(r-1)!} & r = 1, 2, 3, \dots \end{cases}$$

Where, $\psi_n(z)$ is the polygamma function, $B_{n,k}(f_1, f_2, \dots)$ is Bell polynomials, γ_r is Stieltjes constant,

The first few of A_r are

$$A_0 = 1$$

$$A_1 = \frac{\text{Log}[\pi]}{2} - \gamma_0 - \frac{1}{2} \psi_0\left[\frac{3}{2}\right]$$

$$A_2 = \frac{\text{Log}[\pi]^2}{8} - \frac{1}{2} \text{Log}[\pi] \gamma_0 - \gamma_1 - \frac{1}{4} \text{Log}[\pi] \psi_0\left[\frac{3}{2}\right] + \frac{1}{2} \gamma_0 \psi_0\left[\frac{3}{2}\right] + \frac{1}{8} \left(\psi_0\left[\frac{3}{2}\right]^2 + \psi_1\left[\frac{3}{2}\right] \right)$$

$$A_3 = \frac{\text{Log}[\pi]^3}{48} - \frac{1}{8} \text{Log}[\pi]^2 \gamma_0 - \frac{1}{2} \text{Log}[\pi] \gamma_1 - \frac{\gamma_2}{2} - \frac{1}{16} \text{Log}[\pi]^2 \psi_0\left[\frac{3}{2}\right] +$$

$$\frac{1}{4} \text{Log}[\pi] \gamma_0 \psi_0\left[\frac{3}{2}\right] + \frac{1}{2} \gamma_1 \psi_0\left[\frac{3}{2}\right] + \frac{1}{16} \text{Log}[\pi] \left(\psi_0\left[\frac{3}{2}\right]^2 + \psi_1\left[\frac{3}{2}\right] \right) -$$

$$\frac{1}{8} \gamma_0 \left(\psi_0\left[\frac{3}{2}\right]^2 + \psi_1\left[\frac{3}{2}\right] \right) + \frac{1}{48} \left(-\psi_0\left[\frac{3}{2}\right]^3 - 3 \psi_0\left[\frac{3}{2}\right] \psi_1\left[\frac{3}{2}\right] - \psi_2\left[\frac{3}{2}\right] \right)$$

$$A_4 = \frac{\text{Log}[\pi]^4}{384} - \frac{1}{48} \text{Log}[\pi]^3 \gamma_0 - \frac{1}{8} \text{Log}[\pi]^2 \gamma_1 - \frac{1}{4} \text{Log}[\pi] \gamma_2 - \frac{\gamma_3}{6} -$$

$$\frac{1}{96} \text{Log}[\pi]^3 \psi_0\left[\frac{3}{2}\right] + \frac{1}{16} \text{Log}[\pi]^2 \gamma_0 \psi_0\left[\frac{3}{2}\right] + \frac{1}{4} \text{Log}[\pi] \gamma_1 \psi_0\left[\frac{3}{2}\right] + \frac{1}{4} \gamma_2 \psi_0\left[\frac{3}{2}\right] +$$

$$\frac{1}{64} \text{Log}[\pi]^2 \left(\psi_0\left[\frac{3}{2}\right]^2 + \psi_1\left[\frac{3}{2}\right] \right) - \frac{1}{16} \text{Log}[\pi] \gamma_0 \left(\psi_0\left[\frac{3}{2}\right]^2 + \psi_1\left[\frac{3}{2}\right] \right) - \frac{1}{8} \gamma_1 \left(\psi_0\left[\frac{3}{2}\right]^2 + \psi_1\left[\frac{3}{2}\right] \right) +$$

$$\frac{1}{96} \text{Log}[\pi] \left(-\psi_0\left[\frac{3}{2}\right]^3 - 3 \psi_0\left[\frac{3}{2}\right] \psi_1\left[\frac{3}{2}\right] - \psi_2\left[\frac{3}{2}\right] \right) - \frac{1}{48} \gamma_0 \left(-\psi_0\left[\frac{3}{2}\right]^3 - 3 \psi_0\left[\frac{3}{2}\right] \psi_1\left[\frac{3}{2}\right] - \psi_2\left[\frac{3}{2}\right] \right) +$$

$$\frac{1}{384} \left(\psi_0\left[\frac{3}{2}\right]^4 + 6 \psi_0\left[\frac{3}{2}\right]^2 \psi_1\left[\frac{3}{2}\right] + 3 \psi_1\left[\frac{3}{2}\right]^2 + 4 \psi_0\left[\frac{3}{2}\right] \psi_2\left[\frac{3}{2}\right] + \psi_3\left[\frac{3}{2}\right] \right)$$

`Tblpsi[r_, z_] := Table[PolyGamma[k, z], {k, 0, r - 1}]`

`gamma_s_ := StieltjesGamma[s]`

`SetPrecision[{A1, A2, A3, A4}, 14]`

`{-0.0230957089661, 0.0233438645342, -0.0004979838499, 0.0002531817303}`

Combining Lemma 14.2.2 ~ Lemma 14.2.4, we obtain the following theorem.

Theorem 14.2.5

If ρ_{r_1} $r_1 = 1, 2, 3, \dots$ are nontrivial zeros of the Riemann Zeta function $\zeta(z)$, the Li coefficients λ_n $n = 1, 2, 3, \dots$ are expressed as follows.

$$\lambda_n = -nA_1 + \sum_{k=2}^n (-1)^{k-1} \binom{n}{k} \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^k} \quad (\text{When } n = 1, \text{ the 2 rd term is ignored.})$$

$$\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} = -A_1$$

$$\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^k} = (-A_1)^k - 2(-A_1)^{k-2}A_2 - \sum_{s=0}^{k-3} (-A_1)^s \left\{ \sum_{t=2}^{k-s-1} \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^{k-s-t}} \right) A_t + (k-s)A_{k-s} \right\}$$

(When $k \leq 2$, the 3 nd term is ignored.)

A_r , $r=1, 2, 3, \dots$ are determined by the following equation, where $\psi_r(z)$ is a Polygamma function, $B_{r,k}(f_1, f_2, \dots)$ is a Bell polynomial, and γ_s is the Stieltjes constant.

$$A_r = \sum_{s=0}^r \sum_{t=0}^s \frac{\log^{r-s} \pi}{2^{r-s} (r-s)!} \frac{(-1)^{s-t} g_{s-t}(3/2)}{2^{s-t} (s-t)!} h_t \quad (2.5a)$$

$$g_r\left(\frac{3}{2}\right) = \begin{cases} 1 & r = 0 \\ \sum_{k=1}^r B_{r,k}\left(\psi_0\left(\frac{3}{2}\right), \psi_1\left(\frac{3}{2}\right), \dots, \psi_{r-1}\left(\frac{3}{2}\right)\right) & r = 1, 2, 3, \dots \end{cases}$$

$$h_r = \begin{cases} 1 & r = 0 \\ -\frac{\gamma_{r-1}}{(r-1)!} & r = 1, 2, 3, \dots \end{cases}$$

Proof

From Lemma 14.2.1 and Lemma 14.2.2 ,

$$\lambda_n = n \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} + \sum_{k=2}^n (-1)^{k-1} \binom{n}{k} \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^k} \quad (2.1n)$$

$$\begin{aligned} \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^n} &= \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \right)^n - 2 \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \right)^{n-2} H_2 \\ &\quad - \sum_{s=0}^{n-3} \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} \right)^s \left\{ \sum_{t=2}^{n-s-1} (-1)^t \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^{n-s-t}} \right) H_t + (-1)^{n-s} (n-s) H_{n-s} \right\} \end{aligned} \quad (2.2n)$$

$$H_n = \sum_{r_1=1}^{\infty} \sum_{r_2=r_1+1}^{\infty} \sum_{r_3=r_2+1}^{\infty} \dots \sum_{r_n=r_{n-1}+1}^{\infty} \frac{1}{\rho_{r_1} \rho_{r_2} \rho_{r_3} \dots \rho_{r_n}} \quad (2.Hn)$$

From Lemma 14.2.3 ,

$$\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}} = -A_1 \quad (2.3_1)$$

Substituting this for (2.1n) and (2.2n) ,

$$\begin{aligned} \lambda_n &= -nA_1 + \sum_{k=2}^n (-1)^{k-1} \binom{n}{k} \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^k} \\ \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^n} &= (-A_1)^n - 2(-A_1)^{n-2}H_2 \\ &\quad - \sum_{s=0}^{n-3} (-A_1)^s \left\{ \sum_{t=2}^{n-s-1} (-1)^t \left(\sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^{n-s-t}} \right) H_t + (-1)^{n-s} (n-s) H_{n-s} \right\} \end{aligned}$$

From (2.Hn) and Lemm 14.2.3 (2.3n) ,

$$H_n = (-1)^n A_n \quad n=2, 3, 4, \dots$$

Substituting these for the above two expressions, we obtain the desired expressions.

And provisos A_r , g_r , h_r follow from Lemma 14.2.4. Q.E.D.

The statement in Theorem 14.2.5 is easy to read but not suitable for calculations, so we replace the sum of powers with

$$G_1 = -A_1, \quad G_k = \sum_{r_1=1}^{\infty} \frac{1}{\rho_{r_1}^k} \quad k=2, 3, 4, \dots$$

This leads to the following theorem, which is suitable for recursive calculations.

Theorem 14.2.5'

The Li coefficients λ_n $n = 1, 2, 3, \dots$ can be calculated as follows.

$$\lambda_n = -nA_1 + \sum_{k=2}^n (-1)^{k-1} \binom{n}{k} G_k \quad (\text{When } n=1, \text{ the 2nd term is ignored.})$$

$$G_1 = -A_1$$

$$G_k = (-A_1)^k - 2(-A_1)^{k-2}A_2 - \sum_{s=0}^{k-3} (-A_1)^s \left\{ \sum_{t=2}^{k-s-1} G_{k-s-t} A_t + (k-s)A_{k-s} \right\}$$

(When $k \leq 2$, the 3rd term is ignored.)

Where, A_r $r=1, 2, 3, \dots$ are determined by the following expressions when $\psi_r(z)$ is a Polygamma function,

$B_{r,k}(f_1, f_2, \dots)$ is a Bell polynomial, and γ_s is a Stieltjes function.

$$A_r = \sum_{s=0}^r \sum_{t=0}^s \frac{\log^{r-s} \pi}{2^{r-s} (r-s)!} \frac{(-1)^{s-t} g_{s-t}(3/2)}{2^{s-t} (s-t)!} h_t$$

$$g_r\left(\frac{3}{2}\right) = \begin{cases} 1 & r=0 \\ \sum_{k=1}^r B_{r,k}\left(\psi_0\left(\frac{3}{2}\right), \psi_1\left(\frac{3}{2}\right), \dots, \psi_{r-1}\left(\frac{3}{2}\right)\right) & r=1, 2, 3, \dots \end{cases}$$

$$h_r = \begin{cases} 1 & r=0 \\ -\frac{\gamma_{r-1}}{(r-1)!} & r=1, 2, 3, \dots \end{cases}$$

In fact, when this theorem is executed using the mathematical processing software **Mathematica**, it is as follows.

Li coefficients (symbolic) λ_n

$$\lambda_n := -n A_1 + \sum_{k=2}^n (-1)^{k-1} \text{Binomial}[n, k] G_k$$

$$G_1 := -A_1$$

$$G_k := (-A_1)^k - 2(-A_1)^{k-2} A_2 - \sum_{s=0}^{k-3} (-A_1)^s \left(\sum_{t=2}^{k-s-1} G_{k-s-t} A_t + (k-s) A_{k-s} \right)$$

Where,

$$A_r := \sum_{s=0}^r \sum_{t=0}^s \frac{\text{Log}[\pi]^{r-s}}{2^{r-s} (r-s)!} \frac{(-1)^{s-t} g_{s-t}[3/2]}{2^{s-t} (s-t)!} h_t$$

$$g_r\left[\frac{3}{2}\right] := \text{If}\left[r=0, 1, \sum_{k=1}^r \text{BellY}[r, k, \text{Tbl}\psi\left[r, \frac{3}{2}\right]]\right]$$

$$h_r := \text{If}\left[r=0, 1, -\frac{\gamma_{r-1}}{(r-1)!}\right]$$

$$\text{Tbl}\psi[r_, z_] := \text{Table}[\psi_k[z], \{k, 0, r-1\}]$$

$$\begin{aligned}
\text{Expand}[\lambda_1] & -\frac{\text{Log}[\pi]}{2} + \gamma_\theta + \frac{1}{2} \psi_\theta\left[\frac{3}{2}\right] \\
\text{Expand}[\lambda_2] & -\text{Log}[\pi] + 2\gamma_\theta - \gamma_\theta^2 - 2\gamma_1 + \psi_\theta\left[\frac{3}{2}\right] + \frac{1}{4} \psi_1\left[\frac{3}{2}\right] \\
\text{Expand}[\lambda_3] & -\frac{3\text{Log}[\pi]}{2} + 3\gamma_\theta - 3\gamma_\theta^2 + \gamma_\theta^3 - 6\gamma_1 + 3\gamma_\theta\gamma_1 + \frac{3\gamma_2}{2} + \frac{3}{2} \psi_\theta\left[\frac{3}{2}\right] + \frac{3}{4} \psi_1\left[\frac{3}{2}\right] + \frac{1}{16} \psi_2\left[\frac{3}{2}\right] \\
\text{Expand}[\lambda_4] & -2\text{Log}[\pi] + 4\gamma_\theta - 6\gamma_\theta^2 + 4\gamma_\theta^3 - \gamma_\theta^4 - 12\gamma_1 + 12\gamma_\theta\gamma_1 - 4\gamma_\theta^2\gamma_1 - \\
& 2\gamma_1^2 + 6\gamma_2 - 2\gamma_\theta\gamma_2 - \frac{2\gamma_3}{3} + 2\psi_\theta\left[\frac{3}{2}\right] + \frac{3}{2} \psi_1\left[\frac{3}{2}\right] + \frac{1}{4} \psi_2\left[\frac{3}{2}\right] + \frac{1}{96} \psi_3\left[\frac{3}{2}\right] \\
\text{Expand}[\lambda_5] & -\frac{5\text{Log}[\pi]}{2} + 5\gamma_\theta - 10\gamma_\theta^2 + 10\gamma_\theta^3 - 5\gamma_\theta^4 + \gamma_\theta^5 - 20\gamma_1 + 30\gamma_\theta\gamma_1 - \\
& 20\gamma_\theta^2\gamma_1 + 5\gamma_\theta^3\gamma_1 - 10\gamma_1^2 + 5\gamma_\theta\gamma_1^2 + 15\gamma_2 - 10\gamma_\theta\gamma_2 + \frac{5}{2} \gamma_\theta^2\gamma_2 + \frac{5\gamma_1\gamma_2}{2} - \frac{10\gamma_3}{3} + \\
& \frac{5\gamma_\theta\gamma_3}{6} + \frac{5\gamma_4}{24} + \frac{5}{2} \psi_\theta\left[\frac{3}{2}\right] + \frac{5}{2} \psi_1\left[\frac{3}{2}\right] + \frac{5}{8} \psi_2\left[\frac{3}{2}\right] + \frac{5}{96} \psi_3\left[\frac{3}{2}\right] + \frac{1}{768} \psi_4\left[\frac{3}{2}\right] \\
\text{Expand}[\lambda_6] & -3\text{Log}[\pi] + 6\gamma_\theta - 15\gamma_\theta^2 + 20\gamma_\theta^3 - 15\gamma_\theta^4 + 6\gamma_\theta^5 - \gamma_\theta^6 - 30\gamma_1 + 60\gamma_\theta\gamma_1 - 60\gamma_\theta^2\gamma_1 + \\
& 30\gamma_\theta^3\gamma_1 - 6\gamma_\theta^4\gamma_1 - 30\gamma_1^2 + 30\gamma_\theta\gamma_1^2 - 9\gamma_\theta^2\gamma_1^2 - 2\gamma_1^3 + 30\gamma_2 - 30\gamma_\theta\gamma_2 + 15\gamma_\theta^2\gamma_2 - \\
& 3\gamma_\theta^3\gamma_2 + 15\gamma_1\gamma_2 - 6\gamma_\theta\gamma_1\gamma_2 - \frac{3\gamma_2^2}{4} - 10\gamma_3 + 5\gamma_\theta\gamma_3 - \gamma_\theta^2\gamma_3 - \gamma_1\gamma_3 + \frac{5\gamma_4}{4} - \frac{\gamma_\theta\gamma_4}{4} - \\
& \frac{\gamma_5}{20} + 3\psi_\theta\left[\frac{3}{2}\right] + \frac{15}{4} \psi_1\left[\frac{3}{2}\right] + \frac{5}{4} \psi_2\left[\frac{3}{2}\right] + \frac{5}{32} \psi_3\left[\frac{3}{2}\right] + \frac{1}{128} \psi_4\left[\frac{3}{2}\right] + \frac{1}{7680} \psi_5\left[\frac{3}{2}\right]
\end{aligned}$$

Then, giving values to $\psi_n(3/2)$ & γ_n and calculating, we obtain,

Li coefficients (numerical) λ_n

```
Tbl $\psi$ [r_, z_] := Table[PolyGamma[k, z], {k,  $\theta$ , r - 1}]
```

```
 $\gamma_s$ _ := StieltjesGamma[s]
```

```
SetPrecision[{ $\lambda_1$ ,  $\lambda_2$ ,  $\lambda_3$ ,  $\lambda_4$ }, 14]
```

```
{0.0230957089661, 0.092345735228, 0.207638920554, 0.36879047949}
```

These results are consistent with known values (OEIS A074760 , A104539 , A104540 , A104541).

14.3 Components of Li Coefficients

The Li coefficients λ_n obtained in the previous section was as follows.

$$\begin{aligned}\lambda_1 &= -\frac{1}{2} \log \pi + \frac{1}{2} \psi_0\left(\frac{3}{2}\right) + \gamma_0 \\ \lambda_2 &= -\log \pi + \psi_0\left(\frac{3}{2}\right) + \frac{1}{4} \psi_1\left(\frac{3}{2}\right) + 2\gamma_0 - \gamma_0^2 - 2\gamma_1 \\ \lambda_3 &= -\frac{3}{2} \log \pi + \frac{3}{2} \psi_0\left(\frac{3}{2}\right) + \frac{3}{4} \psi_1\left(\frac{3}{2}\right) + \frac{1}{16} \psi_2\left(\frac{3}{2}\right) \\ &\quad + 3\gamma_0 - 3\gamma_0^2 + \gamma_0^3 - 6\gamma_1 + 3\gamma_0\gamma_1 + \frac{3}{2}\gamma_2 \\ \lambda_4 &= -2 \log \pi + 2 \psi_0\left(\frac{3}{2}\right) + \frac{3}{2} \psi_1\left(\frac{3}{2}\right) + \frac{1}{4} \psi_2\left(\frac{3}{2}\right) + \frac{1}{96} \psi_3\left(\frac{3}{2}\right) \\ &\quad + 4\gamma_0 - 6\gamma_0^2 + 4\gamma_0^3 - \gamma_0^4 - 12\gamma_1 + 12\gamma_0\gamma_1 - 4\gamma_0^2\gamma_1 - 2\gamma_1^2 + 6\gamma_2 - 2\gamma_0\gamma_2 - \frac{2}{3}\gamma_3 \\ &\quad \vdots\end{aligned}$$

Looking at these again, we can see that Li coefficient λ_n consist of 3 components, namely, $\log \pi$, the polygamma function $\psi_n(3/2)$ and the Stieltjes constant γ_n . These originate from $\pi^{-z/2}$, $\zeta(z)$ and $\Gamma(1/2)$ respectively. Moreover, these are neatly divided into thirds. There are no terms like $\gamma_2 \log \pi$ or $\gamma_3 \psi_1(3/2)$. Considering that these components were obtained from A_n in Lemma 14.2.4, this is surprising.

Formulatable polynomials μ_n

Among λ_n , polynomials consisting of $\log \pi$ and $\psi_n(3/2)$ seem to be possible to formulate. In fact, we can prove the following formula

Formula 14.3.1

Among Li coefficients λ_n $n=1, 2, 3, \dots$, the polynomial μ_n $n=1, 2, 3, \dots$ consisting of $\log \pi$ and the polygamma function $\psi_n(3/2)$ are given by

$$\mu_n = -\frac{n}{2} \log \pi + \sum_{k=1}^n \frac{n}{2^k k!} \binom{n-1}{k-1} \psi_{k-1}\left(\frac{3}{2}\right) \quad (3.1n)$$

Proof

At a glance, we can see that the monomial of $\log \pi$ is as follows:

$$-\frac{n}{2} \log \pi \quad n=1, 2, 3, \dots$$

So,

$$\begin{aligned}\mu_1 &= -\frac{1}{2} \log \pi + \frac{1}{2} \psi_0\left(\frac{3}{2}\right) \\ \mu_2 &= -\frac{2}{2} \log \pi + \psi_0\left(\frac{3}{2}\right) + \frac{1}{4} \psi_1\left(\frac{3}{2}\right) \\ \mu_3 &= -\frac{3}{2} \log \pi + \frac{3}{2} \psi_0\left(\frac{3}{2}\right) + \frac{3}{4} \psi_1\left(\frac{3}{2}\right) + \frac{1}{16} \psi_2\left(\frac{3}{2}\right)\end{aligned}$$

$$\mu_4 = -\frac{4}{2} \log \pi + 2 \psi_0\left(\frac{3}{2}\right) + \frac{3}{2} \psi_1\left(\frac{3}{2}\right) + \frac{1}{4} \psi_2\left(\frac{3}{2}\right) + \frac{1}{96} \psi_3\left(\frac{3}{2}\right)$$

⋮

Reducing the $\psi_n(3/2)$ terms gives

$$\mu_1 = -\frac{1}{2} \log \pi + \frac{1}{2^1 0!} \left\{ \psi_0\left(\frac{3}{2}\right) \right\}$$

$$\mu_2 = -\frac{2}{2} \log \pi + \frac{1}{2^2 1!} \left\{ 4 \psi_0\left(\frac{3}{2}\right) + \psi_1\left(\frac{3}{2}\right) \right\}$$

$$\mu_3 = -\frac{3}{2} \log \pi + \frac{1}{2^3 2!} \left\{ 24 \psi_0\left(\frac{3}{2}\right) + 12 \psi_1\left(\frac{3}{2}\right) + \psi_2\left(\frac{3}{2}\right) \right\}$$

$$\mu_4 = -\frac{4}{2} \log \pi + \frac{1}{2^4 3!} \left\{ 192 \psi_0\left(\frac{3}{2}\right) + 144 \psi_1\left(\frac{3}{2}\right) + 24 \psi_2\left(\frac{3}{2}\right) + \psi_3\left(\frac{3}{2}\right) \right\}$$

⋮

The integer sequence in $\{ \}$ is

$$1, 4, 1, 24, 12, 1, 192, 144, 24, 1, \dots$$

Searching for this in **On-Line Encyclopedia of Integer Sequences (OEIS)**, **A079621** was found. This is given by

$$T(n, k) = \frac{n!}{k!} \binom{n-1}{k-1} 2^{n-k}$$

Using this, μ_n $n=1, 2, 3, \dots$ can be expressed as

$$\begin{aligned} \mu_n &= -\frac{n}{2} \log \pi + \sum_{k=1}^n \frac{1}{2^n (n-1)!} \frac{n!}{k!} \binom{n-1}{k-1} 2^{n-k} \psi_{k-1}\left(\frac{3}{2}\right) \\ &= -\frac{n}{2} \log \pi + \sum_{k=1}^n \frac{1}{2^n} \frac{n}{k!} \binom{n-1}{k-1} 2^{n-k} \psi_{k-1}\left(\frac{3}{2}\right) \end{aligned}$$

i.e.

$$\mu_n = -\frac{n}{2} \log \pi + \sum_{k=1}^n \frac{n}{2^k k!} \binom{n-1}{k-1} \psi_{k-1}\left(\frac{3}{2}\right)$$

Q.E.D.

When this formula is executed using *Mathematica*, it is as follows.

$$\mu_n := -\frac{n}{2} \text{Log}[\pi] + \sum_{k=1}^n \frac{n}{2^k k!} \text{Binomial}[n-1, k-1] \psi_{k-1}\left[\frac{3}{2}\right]$$

$$\mu_1 = -\frac{\text{Log}[\pi]}{2} + \frac{1}{2} \psi_0\left[\frac{3}{2}\right]$$

$$\mu_2 = -\text{Log}[\pi] + \psi_0\left[\frac{3}{2}\right] + \frac{1}{4} \psi_1\left[\frac{3}{2}\right]$$

$$\mu_3 = -\frac{3 \text{Log}[\pi]}{2} + \frac{3}{2} \psi_0\left[\frac{3}{2}\right] + \frac{3}{4} \psi_1\left[\frac{3}{2}\right] + \frac{1}{16} \psi_2\left[\frac{3}{2}\right]$$

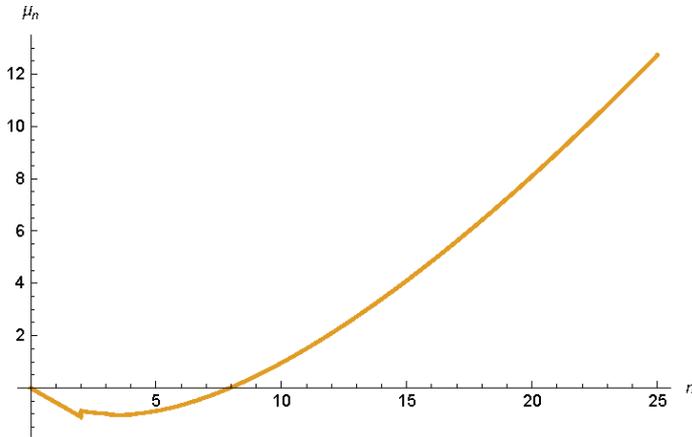
$$\mu_4 = -2 \text{Log}[\pi] + 2 \psi_0\left[\frac{3}{2}\right] + \frac{3}{2} \psi_1\left[\frac{3}{2}\right] + \frac{1}{4} \psi_2\left[\frac{3}{2}\right] + \frac{1}{96} \psi_3\left[\frac{3}{2}\right]$$

$$\mu_5 = -\frac{5 \text{Log}[\pi]}{2} + \frac{5}{2} \psi_0\left[\frac{3}{2}\right] + \frac{5}{2} \psi_1\left[\frac{3}{2}\right] + \frac{5}{8} \psi_2\left[\frac{3}{2}\right] + \frac{5}{96} \psi_3\left[\frac{3}{2}\right] + \frac{1}{768} \psi_4\left[\frac{3}{2}\right]$$

And, giving values to $\psi_n(3/2)$ & γ_n and drawing these,

$$\psi_n\left[\frac{3}{2}\right] := \text{PolyGamma}\left[n, \frac{3}{2}\right]$$

`Plot[μ_n , {n, 0, 25}, AxesLabel -> {n, " μ_n "}, PlotStyle -> ColorData[97, 2]]`



μ_n is negative for $n < 8$ but positive for $n \geq 8$.

Unformulatable polynomials v_n

Among λ_n , denoting the polynomial consisting of γ_n as v_n $n=1, 2, 3, \dots$,

$$v_1 = \gamma_0$$

$$v_2 = 2\gamma_0 - \gamma_0^2 - 2\gamma_1$$

$$v_3 = 3\gamma_0 - 3\gamma_0^2 + \gamma_0^3 - 6\gamma_1 + 3\gamma_0\gamma_1 + \frac{3}{2}\gamma_2$$

$$v_4 = 4\gamma_0 - 6\gamma_0^2 + 4\gamma_0^3 - \gamma_0^4 - 12\gamma_1 + 12\gamma_0\gamma_1 - 4\gamma_0^2\gamma_1 - 2\gamma_1^2 + 6\gamma_2 - 2\gamma_0\gamma_2 - \frac{2}{3}\gamma_3$$

⋮

In conclusion, these formulations are difficult. There is no other way than to use a recurrence relation, as with λ_n in the previous section.

Lemma 14.3.2

Among Li coefficients λ_n $n=1, 2, 3, \dots$, the polynomial v_n $n=1, 2, 3, \dots$ consisting of Stieltjes constants γ_n are given by the following recurrence relation

$$v_n = n\gamma_0 + \sum_{k=2}^n (-1)^{k-1} \binom{n}{k} G_k \quad (\text{When } n=1, \text{ the 2 rd term is ignored.})$$

$$G_1 = \gamma_0$$

$$G_k = \gamma_0^k + 2\gamma_0^{k-2}\gamma_1 + \sum_{s=0}^{k-3} \gamma_0^s \left\{ \sum_{t=2}^{k-s-1} G_{k-s-t} \frac{\gamma_{t-1}}{(t-1)!} + (k-s) \frac{\gamma_{k-s-1}}{(k-s-1)!} \right\}$$

(When $k \leq 2$, the 3 nd term is ignored.)

Proof

Looking at Theorem 14.2.5', the terms consisting only of γ_n contained in $A_1, A_2, A_3, A_4, \dots$ are as follows.

$$-\gamma_0/0!, -\gamma_1/1!, -\gamma_2/2!, -\gamma_3/3!, \dots$$

So, let us insert only $-\gamma_{n-1}/(n-1)!$ into A_n in Theorem 14.2.5' and perform recursive calculation. Then,

$$v_n = -nA_1 + \sum_{k=2}^n (-1)^{k-1} \binom{n}{k} G_k \quad (\text{When } n = 1, \text{ the 2 rd term is ignored.})$$

$$G_1 = -A_1$$

$$G_k = (-A_1)^k - 2(-A_1)^{k-2}A_2 - \sum_{s=0}^{k-3} (-A_1)^s \left\{ \sum_{t=2}^{k-s-1} G_{k-s-t} A_t + (k-s)A_{k-s} \right\}$$

(When $k \leq 2$, the 3 nd term is ignored.)

$$A_r = -\frac{\gamma_{r-1}}{(r-1)!}$$

Substituting the last expression for the above 3 expressions, we obtain the desired expressions. Q.E.D.

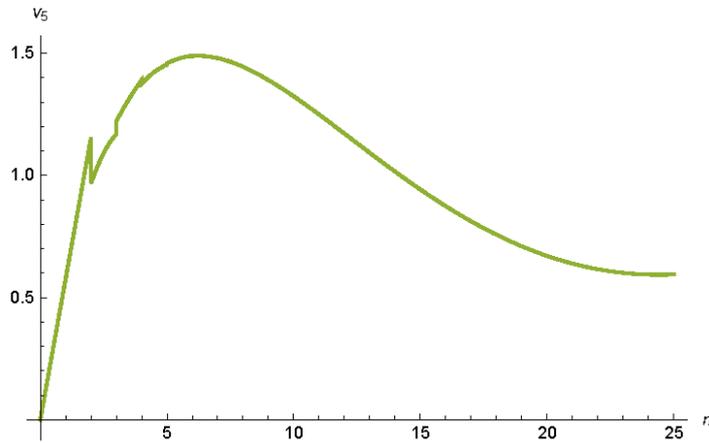
When this Lemma is executed using *Mathematica*, it is as follows.

$$G_1 := \gamma_\theta$$

$$G_{k_} := \gamma_\theta^k + 2\gamma_\theta^{k-2}\gamma_1 + \sum_{s=0}^{k-3} \gamma_\theta^s \left(\sum_{t=2}^{k-s-1} G_{k-s-t} \frac{\gamma_{t-1}}{(t-1)!} + (k-s) \frac{\gamma_{k-s-1}}{(k-s-1)!} \right)$$

$$\gamma_{s_} := \text{StieltjesGamma}[s]$$

`Plot[v_n, {n, 0, 25}, AxesLabel -> {n, "v_s"}, PlotStyle -> ColorData[97, 3]]`



Li Coefficients λ_n

Summarising the above, we obtain the following.

Theorem 14.3.3

When $\psi_r(z)$ is the polygamma function and γ_s is the Stieltjes constant, the Li coefficient λ_n is expressed as follows.

$$\lambda_n = \mu_n + v_n$$

$$\mu_n = -\frac{n}{2} \log \pi + \sum_{k=1}^n \frac{n}{2^k k!} \binom{n-1}{k-1} \psi_{k-1} \left(\frac{3}{2} \right)$$

$$v_n = n\gamma_0 + \sum_{k=2}^n (-1)^{k-1} \binom{n}{k} G_k \quad (\text{When } n = 1, \text{ the 2 rd term is ignored.})$$

Where,

$$G_1 = \gamma_0$$

$$G_k = \gamma_0^k + 2\gamma_0^{k-2}\gamma_1 + \sum_{s=0}^{k-3} \gamma_0^s \left\{ \sum_{t=2}^{k-s-1} G_{k-s-t} \frac{\gamma_{t-1}}{(t-1)!} + (k-s) \frac{\gamma_{k-s-1}}{(k-s-1)!} \right\}$$

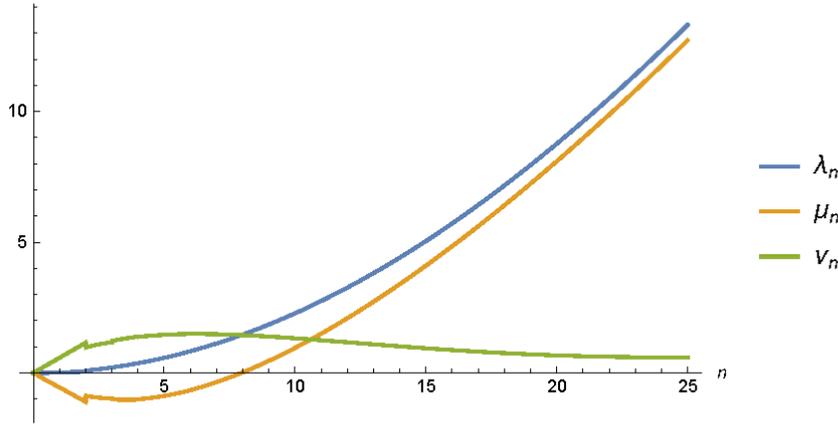
(When $k \leq 2$, the 3 nd term is ignored.)

Executing this using Mathematica, we can obtain the λ_n $n=1, 2, 3, \dots$ at the beginning of this section.

And, giving values to $\psi_n(3/2)$ and γ_n , and drawing λ_n, μ_n, ν_n together, we obtain the following:

$$\lambda_n := \mu_n + \nu_n$$

`Plot[{λn, μn, νn}, {n, 0, 25}, AxesLabel → Automatic, PlotLegends → "Expressions"]`



`SetPrecision[{λ5, λ10, λ15, λ20, λ25}, 14]`

`{0.57554271446, 2.2793393632, 5.04507937, 8.7692769, 13.32098}`

Note

It is wonder that the shapes of μ_n and ν_n are symmetrical up and down at $n < 11$.

We can replace $\psi_n(3/2)$ in μ_n with γ_n and $\log 2$. However, this results in a linear series in γ_n , as follows:

$$\begin{aligned} \mu_n = & -\frac{n}{2} \log \pi + \frac{n}{2} \left(1 - \log 2 - \frac{\gamma_0}{2} \right) + n \sum_{k=2}^n \frac{(-1)^k}{k} \left(\frac{1-2^{-k}}{k-1} \right) \binom{n-1}{k-1} \\ & + n \sum_{k=2}^n \frac{(-1)^k}{k} (1-2^{-k}) \binom{n-1}{k-1} \sum_{s=0}^{\infty} (-1)^s \frac{\gamma_s}{s!} (k-1)^s \end{aligned}$$

The first few are

$$\mu_1 = \frac{1}{2} - \frac{\log 2}{2} - \frac{\log \pi}{2} - \frac{\gamma_0}{4}$$

$$\mu_2 = \frac{3}{4} - \frac{2 \log 2}{2} - \frac{2 \log \pi}{2} + \frac{\gamma_0}{4} - \frac{3\gamma_1}{4} + \frac{3\gamma_2}{8} - \frac{\gamma_3}{8} + \frac{\gamma_4}{32} - \frac{\gamma_5}{160} + \frac{\gamma_6}{960} \dots$$

$$\mu_3 = \frac{21}{16} - \frac{3 \log 2}{2} - \frac{3 \log \pi}{2} + \frac{5\gamma_0}{8} - \frac{\gamma_1}{2} - \frac{5\gamma_2}{8} + \frac{19\gamma_3}{24} - \frac{47\gamma_4}{96} + \frac{103\gamma_5}{480} - \frac{43\gamma_6}{576} \dots$$

$$\mu_4 = \frac{33}{16} - \frac{4 \log 2}{2} - \frac{4 \log \pi}{2} + \frac{15\gamma_0}{16} - \frac{5\gamma_1}{16} - \frac{17\gamma_2}{32} - \frac{29\gamma_3}{96} + \frac{391\gamma_4}{384} - \frac{385\gamma_5}{384} + \frac{7423\gamma_6}{11520} \dots$$

⋮

That is, μ_n is a linear series of γ_n , and ν_n is a polynomial of γ_n . And the shapes of μ_n and ν_n are symmetrical up and down. The above figure is even more puzzling.

14.4 Coffey's Recurrence Relation

According to **Coffey, M. W.** (*Li's Criterion Wolfram MathWorld*), when γ_s is the Stieltjes constant , the Li coefficients λ_n is given by the following recurrence relation.

$$\lambda_n = 1 - \frac{1}{2}n(\gamma_0 + \log \pi + 2\log 2) - \sum_{m=1}^n \binom{n}{m} \eta_{m-1} + \sum_{m=2}^n (-1)^m \binom{n}{m} (1-2^{-m}) \zeta(m)$$

Where,

$$\eta_0 = -\gamma_0$$

$$\eta_n = (-1)^{n-1} \left\{ \frac{n+1}{n!} \gamma_n + \sum_{k=0}^{n-1} \frac{(-1)^{k-1}}{(n-k-1)!} \eta_k \gamma_{n-k-1} \right\}$$

When this is executed using *Mathematica*, it is as follows.

Coffey's recurrence relation (symbolic) λ_n

$$\lambda_{n_} := 1 - \frac{1}{2} n (\gamma_0 + \text{Log}[\pi] + 2 \text{Log}[2]) - \sum_{m=1}^n \text{Binomial}[n, m] \eta_{m-1} + \sum_{m=2}^n (-1)^m \text{Binomial}[n, m] (1 - 2^{-m}) \zeta[m]$$

Where,

$$\eta_0 := -\gamma_0$$

$$\eta_{n_} := (-1)^{n-1} \left(\frac{n+1}{n!} \gamma_n + \sum_{k=0}^{n-1} \frac{(-1)^{k-1}}{(n-k-1)!} \eta_k \gamma_{n-k-1} \right)$$

$$\text{Expand}[\lambda_1] \quad 1 - \text{Log}[2] - \frac{\text{Log}[\pi]}{2} + \frac{\gamma_0}{2}$$

$$\text{Expand}[\lambda_2] \quad 1 - 2 \text{Log}[2] - \text{Log}[\pi] + \gamma_0 - \gamma_0^2 - 2 \gamma_1 + \frac{3 \zeta[2]}{4}$$

$$\text{Expand}[\lambda_3] \quad 1 - 3 \text{Log}[2] - \frac{3 \text{Log}[\pi]}{2} + \frac{3 \gamma_0}{2} - 3 \gamma_0^2 + \gamma_0^3 - 6 \gamma_1 + 3 \gamma_0 \gamma_1 + \frac{3 \gamma_2}{2} + \frac{9 \zeta[2]}{4} - \frac{7 \zeta[3]}{8}$$

$$\text{Expand}[\lambda_4] \quad 1 - 4 \text{Log}[2] - 2 \text{Log}[\pi] + 2 \gamma_0 - 6 \gamma_0^2 + 4 \gamma_0^3 - \gamma_0^4 - 12 \gamma_1 + 12 \gamma_0 \gamma_1 - 4 \gamma_0^2 \gamma_1 - 2 \gamma_1^2 + 6 \gamma_2 - 2 \gamma_0 \gamma_2 - \frac{2 \gamma_3}{3} + \frac{9 \zeta[2]}{2} - \frac{7 \zeta[3]}{2} + \frac{15 \zeta[4]}{16}$$

Coffey's recurrence relation (numeric) λ_n

$$\zeta[n_] := \text{Zeta}[n]$$

$$\gamma_{n_} := \text{StieltjesGamma}[n]$$

$$\text{SetPrecision}[\{\lambda_5, \lambda_{10}, \lambda_{15}, \lambda_{20}, \lambda_{25}\}, 14]$$

$$\{0.57554271446, 2.2793393632, 5.04507937, 8.7692769, 13.32098\}$$

Naturally, these values are completely consistent with those in Theorem 14.3.3 .

Relationship with Theorem 14.3.3

Regarding the representation of λ_n , comparing Theorem 14.3.3 with Coffey's recurrence formula, it is as follows

Theorem 14.3.3

$$\lambda_1 = -\frac{1}{2} \log \pi + \frac{1}{2} \psi_0\left(\frac{3}{2}\right) + \gamma_0$$

$$\lambda_2 = -\log \pi + \psi_0\left(\frac{3}{2}\right) + \frac{1}{4} \psi_1\left(\frac{3}{2}\right) + 2\gamma_0 - \gamma_0^2 - 2\gamma_1$$

$$+ 3\gamma_0 - 3\gamma_0^2 + \gamma_0^3 - 6\gamma_1 + 3\gamma_0\gamma_1 + \frac{3}{2}\gamma_2$$

$$\lambda_4 = -2 \log \pi + 2 \psi_0\left(\frac{3}{2}\right) + \frac{3}{2} \psi_1\left(\frac{3}{2}\right) + \frac{1}{4} \psi_2\left(\frac{3}{2}\right) + \frac{1}{96} \psi_3\left(\frac{3}{2}\right)$$

$$+ 4\gamma_0 - 6\gamma_0^2 + 4\gamma_0^3 - \gamma_0^4 - 12\gamma_1 + 12\gamma_0\gamma_1 - 4\gamma_0^2\gamma_1 - 2\gamma_1^2 + 6\gamma_2 - 2\gamma_0\gamma_2 - \frac{2}{3}\gamma_3$$

Coffey's Recurrence Relation

$$\lambda_1 = 1 - \log 2 - \frac{1}{2} \log \pi + \frac{\gamma_0}{2}$$

$$\lambda_2 = 1 - 2 \log 2 - \log \pi + \gamma_0 - \gamma_0^2 - 2\gamma_1 + \frac{3}{4} \zeta(2)$$

$$\lambda_3 = 1 - 3 \log 2 - \frac{3 \log \pi}{2} + \frac{3\gamma_0}{2} - 3\gamma_0^2 + \gamma_0^3 - 6\gamma_1 + 3\gamma_0\gamma_1 + \frac{3\gamma_2}{2} + \frac{9}{4} \zeta(2) - \frac{7}{8} \zeta(3)$$

$$\lambda_4 = 1 - 4 \log 2 - 2 \log \pi + 2\gamma_0 - 6\gamma_0^2 + 4\gamma_0^3 - \gamma_0^4 - 12\gamma_1 + 12\gamma_0\gamma_1$$

$$- 4\gamma_0^2\gamma_1 - 2\gamma_1^2 + 6\gamma_2 - 2\gamma_0\gamma_2 - \frac{2\gamma_3}{3} + \frac{9}{2} \zeta(2) - \frac{7}{2} \zeta(3) - \frac{15}{16} \zeta(4)$$

In Theorem 14.3.3, λ_n consists of 3 components $\log \pi$, $\psi_n(3/2)$, γ_n .

On the other hand, in Coffey's recurrence relation, λ_n consists of 4 components $\log \pi$, $\log 2$, $\zeta(n)$, γ_n .

Among these, $\log 2$, $\zeta(n)$ arise from the following two relational expressions.

$$\psi_0\left(\frac{3}{2}\right) = 2 - 2 \log 2 - \gamma_0 = 0.036489973\dots$$

$$\psi_{n-1}\left(\frac{3}{2}\right) = (-1)^n (n-1)! (2^n - 1) \zeta(n) - (-1)^n (n-1)! 2^n \quad n=2, 3, 4, \dots$$

The ν_n in Theorem 14.3.3 and the η_n in Coffey's recurrence relation are also the same from the second term onwards.

That is, Theorem 14.3.3 and Coffey's recurrence relation are compatible.

In any case, it is difficult to prove that Li coefficients λ_n are positive. The fluctuations of each term that makes up λ_n are erratic and the deviations are too large. Li's criterion itself is excellent. But a frontal attack on this seems unlikely to succeed.

2025.06.20

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