NOTES ON $\log(\zeta(s))''$

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ABSTRACT. Motivated by the connection to the pair correlation of the Riemann zeros, we investigate the second derivative of the logarithm of the Riemann zeta function, in particular the zeros of this function.

Bogomolny and Keating [4] were the first to observe that the function $(\zeta'(s)/\zeta(s))'$ appears in the pair correlation for the Riemann zeros. Berry and Keating [2] wrote in that context

"The appearance of $\zeta(s)$ indicates an astonishing resurgence property of the zeros: in the pair correlation of high Riemann zeros, the low Riemann zeros appear as resonances."

There has been extensive investigation of the zeros of $\zeta'(s)$ and their connection to the Riemann Hypothesis, via the logarithmic derivative $\zeta'/\zeta(s)$. However there seems to be nothing in the literature about the zeros of the derivative

$$\log(\zeta(s))'' = \left(\frac{\zeta'(s)}{\zeta(s)}\right)' = \frac{\zeta(s)\zeta''(s) - \zeta'(s)^2}{\zeta(s)^2}.$$

The connection to the pair correlation of the Riemann zeros is motivation for further study.

Notation. We let

$$\nu(s) = \zeta(s)\zeta''(s) - \zeta'(s)^2.$$

Elementary facts. Near $s = 1$,

$$\log(\zeta(s))'' = \frac{1}{(s - 1)^2} + O(1).$$

Near a zero $\rho$ of $\zeta(s)$ of order $n_{\rho}$,

$$\log(\zeta(s))'' = \frac{-n_{\rho}}{(s - \rho)^2} + O(1),$$

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1See also the recent work of Rodgers [10], and Ford and Zaharescu [6].
and so \( \nu(s) \) has a zero of order \( 2n_\rho - 2 \). In particular for a simple zero of \( \zeta(s) \), this tells us that \( \nu(\rho) \neq 0 \). There are no other poles. The zeros of \( \log(\zeta(s))'' \) are the zeros of \( \nu(s) \), exclusive of any possible multiple zeros of \( \zeta(s) \).

We have that, for \( \text{Re}(s) > 1 \),

\[
(1) \quad \nu(s) = \sum_n \left( \sum_{d|n} \log(d)^2 - \log(d) \log(n/d) \right) n^{-s}.
\]

With \( \Lambda(n) \) Von Mangoldt’s function, and \( \tau(n) \) the divisor function we have that

\[
\log(\zeta(s))'' = \sum_n \Lambda(n) \log(n)n^{-s}, \quad \zeta(s)^2 = \sum_n \tau(n)n^{-s}.
\]

Thus we also have that

\[
(2) \quad \nu(s) = \sum_n \left( \sum_{d|n} \Lambda(d) \log(d) \tau(n/d) \right) n^{-s}.
\]

We will let \( a(n) \) denote the Dirichlet series coefficients of \( \nu(s) \), given by either (1) and (2). Let

\[
A(x) = \sum_{n<x} a(n).
\]
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We have that for $c > 1$,

$$A(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \nu(w) x^w \frac{1}{w} \, dw.$$  

Moving the contour past the pole at $s = 1$, we have that for $0 < c < 1$

$$A(x) = x \cdot p(\log(x)) + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \nu(w) x^w \frac{1}{w} \, dw,$$

where

$$p(t) = \frac{t^3}{6} + \left(C_0 - \frac{1}{2}\right) t^2 + (1 - 4C_1 - 2C_0) t + 4C_2 + 4C_1 + 2C_0 - 1,$$

with $C_0$ is the Euler constant, and $C_1$ and $C_2$ are Stieltjes constants.

**Lemma.** For $p(t)$ as above

$$A(x) = x \cdot p(\log(x)) + O\left(x^{1/2} \log(x)^2\right),$$

i.e., the integral in (3) is $O(x^{1/2} \log(x)^2)$.

**Proof.** This follows via Euler MacLaurin Summation [7, Appendix B] and the ‘method of the hyperbola’ [7, (2.9)]. In particular, one eventually sees ten different term, each of which may be bounded by 1. So the implied constant may be taken to be equal 10. □

**Functional Equation.** As usual let

$$\chi(s) = 2(2\pi)^{s-1} \sin(\pi s/2) \Gamma(1 - s) = \frac{\pi^{(s-1)/2} \Gamma((1 - s)/2)}{\pi^{-s/2} \Gamma(s/2)}.$$

Differentiating the functional equation $\zeta(s) = \chi(s)\zeta(1 - s)$ we deduce that

$$\nu(s) = \chi^2(s) \left(\nu(1 - s) + \left(\psi'(1 - s) - (\pi/2)^2 \csc(\pi s/2)^2\right)\zeta(1 - s)^2\right).$$

Here $\psi'(s)$ denotes the derivative of the **Digamma** function

$$\psi(s) = \frac{\Gamma'(s)}{\Gamma(s)}.$$

Stirling’s Formula tells us that as $s \to \infty$ in the region $|\arg(s)| \leq \pi - \delta$,

$$\psi'(s) = 1/s + O(1/s^2).$$
We have that
\[ \chi^2(s) \ll t^{1 - 2\sigma} \]
\[ \chi^2(s) \left( \psi'(1 - s) - \left( \frac{\pi}{2} \right)^2 \csc(\pi s/2)^2 \right) \ll t^{-2\sigma}. \]

Thus as \( s \to \infty \) in the region \( |\arg(s)| \leq \pi - \delta \),
\[ \nu(s) = \begin{cases} O(1) & \sigma \geq 1 + \delta > 1 \\ O(t^{1 - 2\sigma}) & \sigma \leq -\delta < 0. \end{cases} \]

From the functional equation
\[ \zeta(1 - s) = 2(2\pi)^{-s} \cos(\pi s/2) \Gamma(s)\zeta(s), \]
we deduce
\[ \log(\zeta(1 - s))'' = -\frac{\pi^2}{4} \sec^2(\pi s/2) + \psi'(s) + \log(\zeta(s))''. \]

**Asymptotics.** With \( a(n) \ll n^\epsilon \) we can estimate the sum of the series for \( n \geq 3 \) to obtain
\[ \log(\zeta(s))'' = \frac{\log(2)^2}{2^s} + O\left( \frac{\exp(-\sigma)}{1 + \epsilon - \sigma} \right) \text{ for } \sigma > 1 + \epsilon. \]

Now \( |\sec^2(\pi s/2)| \ll \exp(-\pi t) \). Thus we have

**Proposition.** As \( s \to \infty \) in a vertical strip \( 1 + \epsilon \leq \sigma < \sigma_0 \),
\[ \log(\zeta(1 - s))'' = \frac{\log(2)^2}{2^s} + O\left( \frac{\exp(-\sigma)}{1 + \epsilon - \sigma} \right) + O\left( \frac{1}{s} \right). \]

On the other hand, if \( t \to \infty \) with \( |s|^2 < 2^\sigma \), then
\[ \log(\zeta(1 - s))'' = \frac{1}{s} + O\left( \frac{1}{s^2} \right). \]
Figure 2. Argument of \( \log(\zeta(s))'' \). On the left, the vertical strip \(-9.5 \leq \sigma \leq 10.5\), and \(0 \leq t \leq 100\). On the right, \(-14.5 \leq \sigma \leq 15.5\), and \(10^4 \leq t \leq 10^4 + 100\). The dotted lines denote \( \sigma = 0 \) and \( \sigma = 1 \).
On the border of these two asymptotic regimes, we will see a cancellation where
\[ \frac{1}{s} \approx -\frac{\log(2)^2}{2^s}, \]
creating zeros of \( \nu(s) \) which we refer to as ASYMPTOTICALLY TRIVIAL OF THE FIRST KIND. Equating modulus and argument, this happens when
\[ 2^\sigma \approx \log(2)^2 \left( \sigma^2 + t^2 \right)^{1/2} \quad \text{or} \quad \sigma \approx \log(t) / \log(2), \]
and also \( \tan(t \log(2)) \approx t / \sigma. \)

With \( \sigma \) and \( t \) positive, both \( \cos(t \log(2)) \) and \( \sin(t \log(2)) \) need to be negative, and since \( \sigma \) is very small compared to \( t \) we deduce that \( t \log(2) \) is slightly larger than \( 2 \pi n + 3 \pi / 2 \) for integer \( n \), or \( t \) is about \( 9.1 n + 6.8 \). One sees eleven examples of these asymptotically trivial zeros to the left of the critical line on the right side of Figure 2. In this strip of height 100 they are as predicted about 9.1 units apart and have real part approximately \( 1 - \log(10^4) / \log(2) \approx -12.2 \).

There is a double pole of
\[ -\frac{\pi^2}{4} \sec^2(\pi(1-s)/2) + \psi'(1-s) \]
at the negative even integers. And (11) implies that as \( s \to \infty \) with \( \arg(s) \) a constant \( \pi/2 - \delta \), \( \arg(\log(\zeta(s)))'' \) is asymptotically constant (in fact, asymptotic to \( \delta \)). By the Argument Principle, \( \nu(s) \) will have, for each negative even integer, a pair of complex conjugate zeros inside the rays \( \arg(s) = \pi \pm \delta \). We refer to these zeros as ASYMPTOTICALLY TRIVIAL OF THE SECOND KIND. Examples in the upper half plane can be seen at the bottom of the left side of Figure 2; more examples can be seen in Figure 3. It would be interesting to understand the asymptotic behavior of the imaginary part of these zeros.

\[ \begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Argument of \( \log(\zeta(s))'' \) in the region \(-30 \leq \sigma \leq 1\), and \( 0 \leq t \leq 5 \).}
\end{figure} \]
Zero free region. From the general theory of Dirichlet series, $\nu(s)$ has a right half plane free of zeros.

**Theorem 1.** For $\Re(s) \geq 4.25$, we have that $\nu(s) \neq 0$.

**Proof.** We have by the triangle inequality

$$|\nu(s)| \geq \frac{a(2)}{2^\sigma} - \sum_{n=3}^{\infty} \frac{a(n)}{n^\sigma}.$$

Via summation by parts and the fact that

$$\lim_{y \to \infty} A(y)y^{-\sigma} = 0,$$

we deduce that, with parameter $x$ to be determined,

$$|\nu(s)| \geq \frac{a(2)}{2^\sigma} - \sum_{n=3}^{x} \frac{a(n)}{n^\sigma} + \frac{A(x)}{x^\sigma} - \sigma \int_{x}^{\infty} A(t)t^{-\sigma-1} dt.$$

Via (4) it will suffice that we satisfy the two inequalities

$$\frac{a(2)}{2^\sigma} - \sum_{n=3}^{x} \frac{a(n)}{n^\sigma} > \frac{1.5}{x^{\sigma/2}},$$

and

$$\frac{A(x)}{x^\sigma} - \sigma \int_{x}^{\infty} p(\log(t))t^{-\sigma} dt - \left| 10 \cdot \sigma \int_{x}^{\infty} \log(t)^2t^{-\sigma-1/2} dt \right| > -\frac{1}{x^{\sigma/2}}.$$

Once $x > 4$ is fixed, $a(2) - \sum_{n=3}^{x} a(n) (2/n)^\sigma$ is an increasing function of $\sigma$, bounded above by $a(2)$, and $(2/\sqrt{x})^\sigma$ is decreasing to 0. Thus if the first inequality holds at $\sigma_0$, it will hold on the interval $[\sigma_0, \infty)$.

Next observe

$$\sigma \int_{x}^{\infty} p(\log(t))t^{-\sigma} dt =$$

$$x^{-\sigma} \left( x \cdot p(\log(x)) + \frac{q_1}{\sigma-1} + \frac{q_2}{(\sigma-1)^2} + \frac{q_3}{(\sigma-1)^3} + \frac{q_4}{(\sigma-1)^4} \right),$$

where the $q_j$ are certain polynomials in $x$ and $\log(x)$ in terms of the Stieltjes constants, positive for $x \geq 4$. Meanwhile

$$10 \cdot \sigma \int_{x}^{\infty} \log(t)^2t^{-\sigma-1/2} dt =$$

$$x^{1/2-\sigma} \left( 10\log(x)^2 + \frac{r_1}{(\sigma-1/2)^2} + \frac{r_2}{(\sigma-1/2)^3} + \frac{r_3}{(\sigma-1/2)^4} \right),$$
for certain \( r_i \), polynomials in \( \log(x) \) with positive coefficients. Thus our second inequality is equivalent to

\[
x^\sigma/2 > x \cdot p(\log(x)) + 10x^{1/2}\log(x)^2 - A(x) + x^{1/2} \left( \frac{4}{\sigma - 1} q_j + \sum_{i=1}^{3} \frac{r_i}{(\sigma - 1/2)^i} \right).
\]

For fixed \( x \geq 4 \), the left side is increasing in \( \sigma \), and the right side is decreasing in \( \sigma \) so again this will hold on an interval \( [\sigma_0, \infty) \). With \( x = 40 \), Mathematica verifies that \( \sigma_0 = 4.25 \) suffices. Furthermore, we deduce that for \( \sigma > 4.25 \),

\[
(12) \quad \frac{a(2)}{2^\sigma} - \sum_{n=3}^{\infty} \frac{a(n)}{n^\sigma} > \frac{.5}{40^{\sigma/2}}.
\]

\( \square \)

The number of zeros for \( \nu(s) \). Let

\[
N_\nu(T) = \# \{ \rho \mid \nu(\rho) = 0, 0 < \text{Im}(\rho) < T, -4 < \text{Re}(\rho) \}.
\]

This count excludes the two flavors of asymptotically trivial zeros described above, except for a \( O(1) \) error.

**Theorem 2.**

\[
N_\nu(T) = 2 \left( \frac{T}{2\pi} \log \left( \frac{T}{2\pi} \right) - \frac{T}{2\pi} \right) - \frac{\log(2)}{\pi} T + O(\log(T)).
\]

**Proof.** Let \( C \) be the boundary (described positively) of the rectangle with vertices \( 5 + i10, 5 + iT, -4 + iT, -4 + i10 \). There are no asymptotically trivial zeros inside \( C \). By the functional equation and the zero free region, the nontrivial zeros are inside \( C \). By the Argument Principle, we need to estimate

\[
\frac{1}{2\pi i} \int_C \frac{d}{ds} \log(\nu(s)) \, ds = \\
\frac{1}{2\pi i} \left\{ \int_{5+i10}^{5+iT} + \int_{5+iT}^{-4+iT} + \int_{-4+i10}^{-4+iT} \right\} \frac{d}{ds} \log(\nu(s)) \, ds \\
= \frac{1}{2\pi i} (I_1 + I_2 + I_3 + I_4).
\]

The integral \( I_1 \) is \( O(1) \). Next, \( I_2 \) is equal

\[
(13) \quad \log \left( \frac{a(2)}{2^s} \right) \bigg|_{5+i10}^{5+iT} + \log \left( 1 + \sum_{n=3}^{\infty} \frac{a(n)}{a(2)} \left( \frac{2}{n} \right)^s \right) \bigg|_{5+i10}^{5+iT}.
\]
Via (12), we see that
\begin{equation}
1 - \sum_{n=3}^{\infty} \frac{a(n)}{a(2)} \left( \frac{2}{n} \right)^{-5} > 0.0025,
\end{equation}
thus
\begin{equation}
\Re \left( 1 + \sum_{n=3}^{\infty} \frac{a(n)}{a(2)} \left( \frac{2}{n} \right)^{5+it} \right) > 0,
\end{equation}
and the argument of the expression inside the second logarithm in (13) is bounded by \( \pm \pi/2 \). From the contribution of the first logarithm in (13) we deduce that
\[ I_2 = -i \log(2) T + O(1). \]
Via a fairly routine argument based on Jensen’s Theorem\(^2\), one sees that \( I_3 = O(\log(T)) \).

Finally, for
\[ I_4 = \int_{-4+iT}^{4+i10} \frac{d}{ds} \log(\nu(s)) \, ds = \int_{-4+iT}^{4+i150} \frac{d}{ds} \log(\nu(s)) \, ds + O(1) \]
we will use the functional equation (5) in the form
\begin{equation}
\nu(s) = \chi^2(s) \nu(1-s) \left( 1 + \left( \psi'(1-s) - (\pi/2)^2 \csc(\pi s/2)^2 \frac{\zeta(1-s)^2}{\nu(1-s)} \right) \right).
\end{equation}
We observe that for \( t \geq 150 \)
\begin{equation}
\left| \psi'(5-it) - (\pi/2)^2 \csc(\pi(4+it)/2)^2 \right| < 1/140
\end{equation}
by the exponential decay of cosecant and the Stirling’s formula asymptotic for \( \psi'(5-it) \). Also
\[
|\log(\zeta(5-it))''| \geq \frac{\log(2)^2}{2^5} - \sum_{n=3}^{\infty} \frac{\Lambda(n) \log(n)}{n^5} \geq 0.0075,
\]
\begin{equation}
\left| \frac{\zeta(5-it)^2}{\nu(5-it)} \right| \leq \frac{1}{0.0075} < 135.
\end{equation}
The product of (17) and (18) is \( < 1 \) in absolute value, and thus
\[
\Re \left( 1 + \left( \psi'(5-it) - (\pi/2)^2 \csc(\pi(4+it)/2)^2 \right) \frac{\zeta(5-it)^2}{\nu(5-it)} \right) > 0,
\]
and the argument of this expression is bounded between \(-\pi/2\) and \(\pi/2\). This implies that on the vertical line \(-4+it, T \geq t \geq 150,\)
\[ \Im(\log(\nu(s))) = \Im(\log(\chi^2(s)\nu(1-s))) + O(1). \]
\[ \text{as in, for example, [3]}\]
And similarly, via (14) and (15) we deduce that on this line,

$$\text{Im}(\log(v(s))) = \text{Im}(\log(\chi^2(s) \log(2)^{2^s - 1})) + O(1).$$

Via Stirling’s formula

$$\arg(\chi^2(s)|_{-4+iT}) = 2T \log(T/2\pi) - 2T + O(1), \quad \text{while}$$

$$\arg(\log(2)^{2^s - 1})|_{-4+iT} = -\log(2)T,$$

so

$$\text{Im}(I_4) = 2T \log(T/2\pi) - 2T - \log(2)T + O(1).$$

□

### Zero density results.

**Proposition.** For $p(t)$ as before

(19) \[ A(x) = x \cdot p(\log(x)) + O_\epsilon \left(x^{1/3+\epsilon}\right). \]

**Proof.** Starting with (5) and (8), the proof very closely follows the $k = 2$ case of [11, Theorem 12.2], i.e. the error estimates for the divisor function. □

**Proposition.** Let \[ \phi(s) = \left(1 - 2^{-s}\right)^4 v(s) \]

The abscissa of convergence $\sigma_c$ for $\phi(s)$ is \( \leq 1/3 \).

**Proof.** The Dirichlet series expansion of $\phi(s)$ is $\sum b(n)n^{-s}$, where, if $2^j | n$,

$$b(n) = \sum_{m=0}^{\min(4,j)} \binom{4}{m} (-2)^m a(n/2^m).$$

With $B(x) = \sum_{n \leq x} b(n)$, we have that

$$B(x) = \sum_{m=0}^{4} \binom{4}{m} (-2)^m \sum_{\substack{k \leq x \\text{2^m | k}}} a(k/2^m)$$

$$= \sum_{m=0}^{4} \binom{4}{m} (-2)^m \sum_{n \leq x/2^m} a(n).$$
Via (19) we see that
\[
B(x) = \sum_{m=0}^{4} \binom{4}{m} (-2)^m \left(\frac{x}{2^m} \cdot p(\log(x) - m \log(2)) + O_\epsilon \left(x^{1/3+\epsilon}\right)\right)
\]
\[= x \cdot \sum_{m=0}^{4} \binom{4}{m} (-1)^m p(\log(x) - m \log(2)) + O_\epsilon \left(x^{1/3+\epsilon}\right).\]

With the shift operator \(E_p(t) = p(t - \log(2))\) and difference operator \(\Delta p = (I - E)p\), the main term is \(x \cdot \Delta 4p(\log(x)) = 0\), as \(p\) has degree three and \(\Delta\) reduces the degree. Thus
\[B(x) = O_\epsilon \left(x^{1/3+\epsilon}\right),\]
and so for every \(\epsilon > 0\),
\[
\limsup_{x \to \infty} \frac{\log |B(x)|}{\log(x)} \leq \limsup_{x \to \infty} \frac{(1/3 + \epsilon) \log(x) + \log(C(\epsilon))}{\log(x)} \leq \frac{1}{3} + \epsilon,
\]
and so by [7, Theorem 1.3], we obtain \(\sigma \leq 1/3\). \(\Box\)

**Theorem 3.** If for positive \(\delta\) we denote by \(N_{5/6+\delta}(T)\) the number of zeros of \(\nu(s)\) in the region \(|\text{Im}(s)| \leq T, 5/6 + \delta < \text{Re}(s)\), then
\[
N_{5/6+\delta}(T) \ll_\delta T.
\]

**Proof.** The zeros of \(\nu(s)\) coincide with the zeros of \(\phi(s)\). We will imitate the proof of [8, Theorem 6.18]. For \(x_0 > 4.25\), and any integer \(m\), set \(K_{r,m}\) to be the circle with center \(s_0 = x_0 + (1/2 + m)i\) and radius \(r = |x_0 - 5/6 - \delta + i/2|\). The circle passes through \(5/6 + \delta + mi\) and \(5/6 + \delta + (m + 1)i\). Increasing \(x_0\) if necessary, the circle lies to the right of the line \(\text{Re}(s) = 5/6 + \delta/2\). Set \(K_{R,m}\) to be the circle with center \(s_0 = x_0 + (1/2 + m)i\) and radius \(R = x_0 - 5/6 - \delta/2\). Finally let
\[
A = A(x_0) = 2 \inf_{\text{Re}(s) = x_0} |\phi(s)|.
\]
The proof of Theorem 1 implies \(A > 0\). Now [8, Corollary 2, p.260], a corollary to Jensen’s Theorem, implies there exists \(C = C(r, R, A)\) such that the number of zeros of \(\phi(s)\) in the rectangle
\[
5/6 + \delta \leq \text{Re}(s) \leq x_0, \quad m < \text{Im}(s) \leq m + 1
\]
does not exceed
\[ C \cdot \left| \int_{K_{R,m}} |\phi(x + iy)|^2 \, dx \, dy \right| \leq \]
\[ C \cdot \int_{x_0+R}^{x_0+R} \int_{m+1/2+R}^{m+1/2+R} |\phi(x + iy)|^2 \, dy \, dx. \]

Summing over integers \( m \in [-T, T] \) we deduce that
\[ N_{5/6+\delta}(T) = O \left( \int_{5/6+\delta/2}^{T+1/2+R} \int_{-T+1/2-R}^{T+1/2+R} |\phi(x + iy)|^2 \, dy \, dx \right). \]

The Proposition above, and a theorem of Bohr [5] shows the abscissa of uniform convergence of \( \phi(s) \) is \( \leq 5/6 \). From this and [8, Corollary, p. 315], we deduce that
\[ \int_{x_0+R}^{x_0+R} \int_{-T+1/2-R}^{T+1/2+R} |\phi(x + iy)|^2 \, dy \, dx \ll \delta T. \]

\[ \square \]

Appendix: Numerical methods. The graphics in Figures 2 and 3 require the numerical computation of \( \zeta(s)\zeta''(s) - \zeta'(s)^2 \) on a large grid of points in the complex plane. Numerical computation of derivatives of a function \( f(x) \) is often done by a method called Richardson extrapolation [9, §5.7]. One has that
\[ \frac{f(x + h) - f(x - h)}{2h} = f'(x) + \frac{1}{6} f^{(3)}(x) h^2 + O(h^4), \]
\[ \frac{f(x + 2h) - f(x - 2h)}{4h} = f'(x) + \frac{2}{3} f^{(3)}(x) h^2 + O(h^4), \]
so an appropriate linear combination of the left sides of the two equations computes \( f'(x) \) up to an error \( O(h^4) \). This can be readily generalized to computing each value on a rectangular grid of points of \( \zeta(s)\zeta''(s) - \zeta'(s)^2 \), up to an error \( O(h^8) \), with (asymptotically) a single evaluation of \( \zeta(s) \). One uses the saved function values at \( \zeta(s \pm h) \), \( \zeta(s \pm ih) \), \( \zeta(s + (\pm h \pm ih)) \), as well as \( \zeta(s) \), and the solution to a linear system of 9 equations in 9 unknowns.

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