A NEW UPPER BOUND ON THE LARGEST NORMALIZED LAPLACIAN EIGENVALUE

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Abstract. Let \mathscr{G} be a simple undirected connected graph on n vertices. Suppose that the vertices of \mathscr{G} are labelled $1, 2, \ldots, n$. Let d_i be the degree of the vertex i. The Randić matrix of \mathscr{G} , denoted by R, is the $n \times n$ matrix whose (i, j) – entry is $\frac{1}{\sqrt{d_i d_j}}$ if the vertices i and j are adjacent and 0 otherwise. The normalized Laplacian matrix of \mathscr{G} is $\mathscr{L} = I - R$, where I is the $n \times n$ identity matrix. In this paper, by using an upper bound on the maximum modulus of the subdominant Randić eigenvalues of \mathscr{G} , we obtain an upper bound on the largest eigenvalue of \mathscr{L} . We also obtain an upper bound on the largest eigenvalue of \mathscr{L} .

1. Introduction

Let $\mathscr{G} = (V, E)$ be a simple undirected graph on *n* vertices. Some matrices on \mathscr{G} are the adjacency matrix *A*, the Laplacian matrix L = D - A and the signless Laplacian matrix Q = D + L, where *D* is the diagonal matrix of vertex degrees. It is well known that *L* and *Q* are positive semidefinite matrices and that (0,1) is an eigenpair of *L* where **1** is the all ones vector. Fiedler [16] proved that \mathscr{G} is a connected graph if and only if the second smallest eigenvalue of *L* is positive. This eigenvalue is called the algebraic connectivity of \mathscr{G} . The signless Laplacian matrix has recently attracted the attention of several researchers. Recent papers on this matrix are [5, 6, 7, 8, 9] and some of its basic properties [6] are:

- 1. For a connected graph, the smallest eigenvalue of Q is equal to 0 if and only if the graph is bipartite. In this case, 0 is a simple eigenvalue. Then, for a connected graph, the smallest eigenvalue of Q is positive if and only if the graph is not bipartite.
- 2. If \mathscr{G} is a bipartite graph then Q and L have the same characteristic polynomial.

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Other matrices on the graph \mathscr{G} are the normalized Laplacian matrix and the Randić matrix of \mathscr{G} . Suppose that the vertices of \mathscr{G} are labelled 1, 2, ..., n. Let d_i be the degree of the vertex *i*. Let $D^{-\frac{1}{2}}$ be the diagonal matrix whose diagonal entries are

$$\frac{1}{\sqrt{d_1}}, \frac{1}{\sqrt{d_2}}, \dots, \frac{1}{\sqrt{d_n}}$$

whenever $d_i \neq 0$. If $d_i = 0$ for some *i* then the corresponding diagonal entry of $D^{-\frac{1}{2}}$ is defined to be 0. The normalized Laplacian matrix of \mathscr{G} , denoted by \mathscr{L} , was introduced by F. Chung [15] as

$$\mathscr{L} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}} = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}.$$
 (1)

The eigenvalues of \mathscr{L} are called the normalized Laplacian eigenvalues of \mathscr{G} . From (1), we have

$$D^{\frac{1}{2}}\mathcal{L}D^{\frac{1}{2}} = D - A = L$$

and thus

$$D^{\frac{1}{2}}\mathscr{L}D^{\frac{1}{2}}\mathbf{1} = L\mathbf{1} = 0\mathbf{1}.$$

Hence 0 is an eigenvalue of \mathscr{L} with eigenvector $D^{\frac{1}{2}}\mathbf{1}$.

We recall the following results on \mathscr{L} [15] :

- 1. The eigenvalues of \mathscr{L} lie in the interval [0,2].
- 2. 0 is a simple eigenvalue of \mathscr{L} if and only if \mathscr{G} is connected.
- 3. 2 is an eigenvalue of \mathscr{L} if and only if a connected component of \mathscr{G} is bipartite and nontrivial.

Among papers on \mathcal{L} , we mention [10, 11, 13, 14] and [17].

From now on, we assume that \mathscr{G} is connected graph. Then $d_i > 0$ for all *i*. The notation $i \sim j$ means that the vertices *i* and *j* are adjacent. The matrix $R = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ in (1) is the Randić matrix of \mathscr{G} in which the (i, j)-entry is $\frac{1}{\sqrt{d_i d_j}}$ if $i \sim j$ and 0 otherwise. Moreover

$$I - \mathscr{L} = R.$$

The eigenvalues of R are called the Randić eigenvalues of \mathcal{G} . Clearly \mathcal{L} and R are both real symmetric matrices. The Randić matrix was earlier studied in connection with the Randić index [1, 2, 18] and [19]. Two recent papers on the Randić matrix are [3] and [4].

Throughout this paper

 $0=\lambda_n\leqslant\lambda_{n-1}\leqslant\ldots\leqslant\lambda_1$

and

$$\rho_n \leqslant \rho_{n-1} \leqslant \ldots \leqslant \rho_1$$

are the normalized Laplacian eigenvalues and the Randić eigenvalues of \mathscr{G} , respectively. It follows that

$$\lambda_i = 1 - \rho_{n-i+1} \ (1 \leq i \leq n) \,.$$

If *M* is a nonnegative matrix then, by the Perron-Frobenius Theorem, *M* has an eigenvalue equal to its spectral radius, called the Perron root of *M*. In addition, if *M* is irreducible then the Perron root of *M* is a simple eigenvalue with a corresponding positive eigenvector, called the Perron vector of *M*. Since \mathscr{G} is a connected graph, Randić matrix of \mathscr{G} is a irreducible nonnegative matrix. Let $\mathbf{v} = D^{\frac{1}{2}}\mathbf{1}$. Then $\mathbf{v} = \left[\sqrt{d_1}, \sqrt{d_2}, \dots, \sqrt{d_n}\right]^T$. An easy computation shows that

$$R\mathbf{v} = \mathbf{v}$$

Hence, 1 and \mathbf{v} are the Perron root and the Perron vector of R, respectively.

Let Δ and δ be the largest and smallest vertex degrees of \mathscr{G} , respectively, and let q_n be the smallest eigenvalue of Q.

A recent result involving the largest eigenvalue of \mathscr{L} and the smallest eigenvalue of Q is

THEOREM 1. [17] Let \mathscr{G} be a connected graph. Then

$$2 - \frac{q_n}{\delta} \leqslant \lambda_1 \leqslant 2 - \frac{q_n}{\Delta}.$$
 (2)

We may consider $2 - \frac{q_n}{\Delta}$ as an upper bound on λ_1 . Observe that $2 - \frac{q_n}{\Delta} = 2$ if and only if \mathscr{G} is a bipartite graph.

In this paper, we search for a new upper bound on λ_1 not exceeding the trivial upper bound 2.

2. Searching for an upper bound on λ_1

Since $\sum_{i=1}^{n} \rho_i = tr(R) = 0$, it follows that $\rho_n < 0$. We have

$$\lambda_1 = 1 - \rho_n = 1 + |\rho_n|$$
.

In order to find an upper bound on λ_1 not exceeding 2, we look for an upper bound on $|\rho_n|$ not exceeding 1.

An eigenvalue of a nonnegative matrix M which is different from the Perron root is called a subdominant eigenvalue of M. Let $\xi(M)$ be the maximum modulus of the subdominant eigenvalues of M. Special attention has been devoted to find upper bounds on $\xi(M)$. In [20], we can find a unified presentation of results concerning upper bounds on $\xi(M)$. These upper bounds are important because $\xi(M)$ plays a major role in convergence properties of powers of M. Since

$$\lambda_1 \leqslant 1 + \xi(R), \tag{3}$$

we focus our attention on upper bounds on $\xi(R)$. We recall the result [12, p. 295] :

THEOREM 2. If $M = (m_{i,j}) \ge 0$ of order $n \times n$ has a positive eigenvector

$$\mathbf{w} = [w_1, w_2, \dots, w_n]^T$$

corresponding to the spectral radius $\rho(M)$ of M then

$$\xi\left(M\right) \leqslant \frac{1}{2} \max_{i < j} \sum_{k=1}^{n} w_k \left| \frac{m_{i,k}}{w_i} - \frac{m_{j,k}}{w_j} \right|.$$

where the maximum is taken over all pairs (i, j), $1 \le i < j \le n$.

In order to apply Theorem 2, it is convenient to observe that the Randić matrix of \mathscr{G} is diagonally similar to the row stochastic matrix

$$S = D^{-\frac{1}{2}} R D^{\frac{1}{2}}.$$
 (4)

The following lemma gives some immediate properties of S.

LEMMA 1. 1. The (i, j) – entry of S is $\frac{1}{d_i}$ if $j \sim i$ and 0 otherwise.

2. S1 = 1 where 1 is the all ones vector.

3. **u** is an eigenvector for R corresponding to the eigenvalue α if and only if $D^{-\frac{1}{2}}$ **u** is an eigenvector for S corresponding to the eigenvalue α .

4. If \mathscr{G} is an r-regular graph then S = R.

Let N_i be the set of neighbours of the vertex v_i and let $|N_i|$ be the cardinality of N_i .

THEOREM 3. Let \mathscr{G} be a simple undirected connected graph. If λ_1 is the largest eigenvalue of \mathscr{L} then

$$|\lambda_1| \leqslant 2 - \min_{i < j} \left\{ \frac{|N_i \cap N_j|}{\max\left\{d_i, d_j\right\}} \right\}$$
(5)

where the minimum is taken over all pairs (i, j), $1 \le i < j \le n$.

Proof. We know that the Randić matrix of \mathscr{G} is similar to the row stochastic matrix *S* defined in (4). Then $\xi(R) = \xi(S)$. The eigenvector corresponding to the spectral of *S* is $\mathbf{w} = \mathbf{1}$. Applying Theorem 2 to $S = (s_{i,j})$, we have

$$\begin{split} \xi\left(S\right) &\leqslant \frac{1}{2} \max_{i < j} \sum_{k=1}^{n} \left| s_{i,k} - s_{j,k} \right| \\ &= \frac{1}{2} \max_{i < j} \left(\sum_{k \in N_{i} - N_{j}} \frac{1}{d_{i}} + \sum_{k \in N_{j} - N_{i}} \frac{1}{d_{j}} + \sum_{k \in N_{i} \cap N_{j}} \left| \frac{1}{d_{i}} - \frac{1}{d_{j}} \right| \right) \\ &= \frac{1}{2} \max_{i < j} \left(\frac{\left| N_{i} - N_{j} \right|}{d_{i}} + \frac{\left| N_{j} - N_{i} \right|}{d_{j}} + \sum_{k \in N_{i} \cap N_{j}} \left| \frac{1}{d_{i}} - \frac{1}{d_{j}} \right| \right) \\ &= \frac{1}{2} \max_{i < j} \left(2 - \frac{\left| N_{i} \cap N_{j} \right|}{d_{i}} - \frac{\left| N_{j} \cap N_{i} \right|}{d_{j}} + \sum_{k \in N_{i} \cap N_{j}} \left| \frac{1}{d_{i}} - \frac{1}{d_{j}} \right| \right) \end{split}$$

Suppose $d_i = \max \{d_i, d_j\}$. In this case

$$2 - \frac{|N_i \cap N_j|}{d_i} - \frac{|N_j \cap N_i|}{d_j} + \sum_{k \in N_i \cap N_j} \left| \frac{1}{d_i} - \frac{1}{d_j} \right|$$
$$= 2 - \frac{|N_i \cap N_j|}{d_i} - \frac{|N_j \cap N_i|}{d_j} + \left(\frac{1}{d_j} - \frac{1}{d_i}\right) N_i \cap N_j$$
$$= 2 - \frac{2|N_i \cap N_j|}{d_i}.$$

Similarly, if $d_j = \max \{d_i, d_j\}$ then

$$2 - \frac{\left|N_i \cap N_j\right|}{d_i} - \frac{\left|N_j \cap N_i\right|}{d_j} + \sum_{k \in N_i \cap N_j} \left|\frac{1}{d_i} - \frac{1}{d_j}\right|$$
$$= 2 - \frac{2\left|N_j \cap N_i\right|}{d_j}.$$

Hence

$$\begin{split} \xi\left(S\right) &\leqslant \frac{1}{2} \max_{i < j} \sum_{k=1}^{n} \left| s_{i,k} - s_{j,k} \right| \\ &= \frac{1}{2} \max_{i < j} \left\{ 2 - \frac{2 \left| N_{j} \cap N_{i} \right|}{\max\left\{ d_{i}, d_{j} \right\}} \right\} \\ &= 1 - \min_{i < j} \left\{ \frac{\left| N_{i} \cap N_{j} \right|}{\max\left\{ d_{i}, d_{j} \right\}} \right\} \end{split}$$

Since $\lambda_1 \leq 1 + \xi(R) = 1 + \xi(S)$, the upper bound in (5) follows. \Box

REMARK 1. If \mathscr{G} is a bipartite graph then $|N_i \cap N_j| = 0$, for some i < j, and consequently the upper bound in (5) is equal to 2. This is sufficient condition but it is not a necessary condition. In fact, there are other instances in which $N_i \cap N_j = 0$ for some i < j. One of them is given by a nonbipartite graph having a bridge. However, if $\min_{i < j} |N_i \cap N_j| \ge 1$ and $q_n < 1$ then

$$2 - \min_{i < j} \left\{ \frac{\left| N_i \cap N_j \right|}{\max\left\{ d_i, d_j \right\}} \right\} < 2 - \frac{q_n}{\Delta}.$$
 (6)

In fact

$$q_n < 1 \leq |N_i \cap N_j|$$
 for $i < j$

and

$$\frac{q_n}{\Delta} \leqslant \frac{1}{\max\left\{d_i, d_j\right\}} \text{ for } i < j$$

Then

$$\frac{q_n}{\Delta} < \frac{|N_i \cap N_j|}{\max\left\{d_i, d_j\right\}} \text{ for } i < j.$$

It follows

$$2 - \frac{q_n}{\Delta} > 2 - \min_{i < j} \frac{\left| N_i \cap N_j \right|}{\max\left\{ d_i, d_j \right\}}.$$

Hence, if $\min_{i < j} |N_i \cap N_j| \ge 1$ and $q_n < 1$ then (5) gives a better upper bound for λ_1 than the second inequality in (2) does.

3. Improving the upper bound on λ_1

We have

$$\lambda_1 = u1 + |q_n| \le 1 + \xi(R) = 1 + \xi(S)$$

The upper bound on λ_1 in (5) was obtained by using an upper bound on $\xi(R)$. In this section, in order to get an improved upper bound on λ_1 , we search for an upper bound on $|q_n|$, that is, on the largest modulus of the negative Randić eigenvalues.

THEOREM 4. Let \mathscr{G} be a simple undirected connected graph. If ρ_n is eigenvalue with the largest modulus among the negative Randić eigenvalues of \mathscr{G} then

$$|
ho_n| \leqslant 1 - \min_{i \sim j} \left\{ rac{|N_i \cap N_j|}{\max\left\{d_i, d_j
ight\}}
ight\}$$

where the minimum is taken over all pairs (i, j), $1 \le i < j \le n$, such that the vertices i and j are adjacent.

Proof. Let ρ_n be the largest modulus of the negative Randić eigenvalues of \mathscr{G} . Let

$$\mathbf{x} = [x_1, x_2, \dots, x_n]^T$$

be such that

$$S\mathbf{x} = \rho_n \mathbf{x}.\tag{7}$$

From Lemma 1, we have $\mathbf{x} = D^{-\frac{1}{2}}\mathbf{u}$ where $R\mathbf{u} = \rho_n \mathbf{u}$. Since \mathbf{u} is orthogonal to the Perron vector $\mathbf{v} = \left[\sqrt{d_1}, \sqrt{d_2}, \dots, \sqrt{d_n}\right]^T$, the vector \mathbf{u} has at least one positive component and at least one negative component. Since $\mathbf{x} = D^{-\frac{1}{2}}\mathbf{u}$, this is also true for the vector \mathbf{x} . Let

$$\max\{x_1, x_2, \ldots, x_n\} = x_i$$

and let

$$x_j = \min\{x_k : k \sim i\}$$

Since **x** has at least one positive component, $x_i > 0$. Let $S = (s_{i,j})$. From (7)

$$\rho_n x_j = \sum_{k=1}^n s_{j,k} x_k = \frac{1}{d_j} \sum_{k \in N_j} x_k$$
(8)

and

$$\rho_n x_i = \sum_{k=1}^n s_{i,k} x_k = \frac{1}{d_i} \sum_{k \in N_i} x_k.$$
(9)

Subtracting (9) from (8), we get

$$\rho_n(x_j - x_i) = \frac{1}{d_j} \sum_{k \in N_j} x_k - \frac{1}{d_i} \sum_{k \sim i} x_k.$$

Then

$$q_n(x_j - x_i)$$

$$= \frac{1}{d_j} \sum_{k \in N_j - N_i} x_k + \frac{1}{d_j} \sum_{k \in N_j \cap N_i} x_k - \frac{1}{d_i} \sum_{k \in N_i - N_j} x_k - \frac{1}{d_i} \sum_{k \in N_j \cap N_i} x_k.$$
(10)

By definition, $x_j \leq x_k$ for all $k \sim i$ and $x_k \leq x_i$ for all k. Hence

$$\sum_{k \in N_j - N_i} x_k \leqslant \left| N_j - N_i \right| x_i \tag{11}$$

and

$$-\sum_{k\in N_i-N_j} x_k \leqslant -\left|N_i - N_j\right| x_j.$$
⁽¹²⁾

Replacing the inequalities (11) and (12) in (10), we obtain

$$q_n (x_j - x_i) \\ \leqslant \frac{1}{d_j} |N_j - N_i| x_i - \frac{1}{d_i} |N_i - N_i| x_j + \sum_{k \in N_j \cap N_i} \left(\frac{1}{d_j} - \frac{1}{d_i}\right) x_k.$$

Thus

$$\begin{split} q_n \left(x_j - x_i \right) &\leqslant \frac{1}{2} \frac{1}{d_j} \left| N_j - N_i \right| \left(x_i - x_j \right) + \frac{1}{2} \frac{1}{d_i} \left| N_i - N_j \right| \left(x_i - x_j \right) \\ &+ \frac{1}{2} \left(\frac{1}{d_j} \left| N_j - N_i \right| - \frac{1}{d_i} \left| N_i - N_j \right| \right) \left(x_i + x_j \right) \\ &+ \sum_{k \in N_i \cap N_j} \left(\frac{1}{d_j} - \frac{1}{d_i} \right) x_k. \end{split}$$

Clearly

$$\frac{1}{d_j}\left|N_j - N_i\right| - \frac{1}{d_i}\left|N_i - N_j\right| = \left(\frac{1}{d_i} - \frac{1}{d_j}\right)\left|N_i \cap N_j\right|.$$

Hence

$$\begin{split} \rho_n(x_j - x_i) &\leqslant \frac{1}{2} \frac{1}{d_j} \left| N_j - N_i \right| (x_i - x_j) + \frac{1}{2} \frac{1}{d_i} \left| N_i - N_j \right| (x_i - x_j) \\ &+ \frac{1}{2} \left(\frac{1}{d_i} - \frac{1}{d_j} \right) \left| N_i \cap N_j \right| (x_i + x_j) + \frac{1}{2} \sum_{k \in N_i \cap N_j} \left(\frac{1}{d_j} - \frac{1}{d_i} \right) (x_k + x_k) \\ &= \frac{1}{2} \frac{1}{d_j} \left| N_j - N_i \right| (x_i - x_j) + \frac{1}{2} \frac{1}{d_i} \left| N_i - N_j \right| (x_i - x_j) \\ &+ \frac{1}{2} \sum_{k \in N_i \cap N_j} \left(\frac{1}{d_i} - \frac{1}{d_j} \right) (x_i - x_k + x_j - x_k). \end{split}$$

Moreover

$$\begin{split} &\sum_{k\in N_i\cap N_j} \left(\frac{1}{d_i} - \frac{1}{d_j}\right) (x_i - x_k + x_j - x_k) \\ &\leqslant \sum_{k\in N_i\cap N_j} \left|\frac{1}{d_i} - \frac{1}{d_j}\right| (x_i - x_k) + \sum_{k\in N_i\cap N_j} \left|\frac{1}{d_i} - \frac{1}{d_j}\right| (x_k - x_j) \\ &= \sum_{k\in N_i\cap N_j} \left|\frac{1}{d_i} - \frac{1}{d_j}\right| (x_i - x_j) \,. \end{split}$$

Therefore

$$\rho_{n}(x_{j} - x_{i}) \leq \frac{1}{2} \frac{1}{d_{j}} |N_{j} - N_{i}| (x_{i} - x_{j}) + \frac{1}{2} \frac{1}{d_{i}} |N_{i} - N_{j}| (x_{i} - x_{j})$$

$$+ \frac{1}{2} \sum_{k \in N_{i} \cap N_{j}} \left| \frac{1}{d_{i}} - \frac{1}{d_{j}} \right| (x_{i} - x_{j}).$$

$$(13)$$

If $x_j = x_i$ then $x_k = x_i$ for all $k \sim i$. Consequently, from $S\mathbf{x} = \rho_n \mathbf{x}$, we have

$$q_n x_i = \sum_{k \in N_i} \frac{1}{d_i} x_k = \frac{1}{d_i} \sum_{k \in N_i} x_i = \frac{x_i}{d_i} d_i = x_i.$$

Thus $\rho_n = 1$, which is a contradiction. Hence $x_i - x_j > 0$. Dividing both sides of (13) by $(x_i - x_j)$, we obtain

$$-\rho_n \leqslant \frac{1}{2} \frac{1}{d_j} \left| N_j - N_i \right| + \frac{1}{2} \frac{1}{d_i} \left| N_i - N_j \right| + \frac{1}{2} \sum_{k \in N_i \cap N_j} \left| \frac{1}{d_i} - \frac{1}{d_j} \right|.$$
(14)

As in the proof of Theorem 3, we get

$$\frac{1}{2} \frac{1}{d_j} |N_j - N_i| + \frac{1}{2} \frac{1}{d_i} |N_i - N_j| + \frac{1}{2} \sum_{k \in N_i \cap N_j} \left| \frac{1}{d_i} - \frac{1}{d_j} \right|$$
$$= 1 - \frac{|N_i \cap N_j|}{\max\{d_i, d_j\}}.$$

Consequently

$$|
ho_n| \leqslant 1 - rac{\left|N_i \cap N_j
ight|}{\max\left\{d_i, d_j
ight\}}$$

Observe that the vertices v_i and v_j are adjacent. Hence

$$|\rho_n| \leq \max_{i \sim j} \left\{ 1 - \frac{|N_i \cap N_j|}{\max\left\{d_i, d_j\right\}} \right\} = 1 - \min_{i \sim j} \left\{ \frac{|N_i \cap N_j|}{\max\left\{d_i, d_j\right\}} \right\}.$$

The proof is complete. \Box

Finally, we have

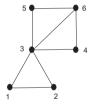
THEOREM 5. Let \mathscr{G} be a simple undirected connected graph. If λ_1 is the largest normalized Laplacian eigenvalue of \mathscr{G} then

$$\lambda_1 \leqslant 2 - \min_{i \sim j} \left\{ rac{\left| N_i \cap N_j
ight|}{\max\left\{ d_i, d_j
ight\}}
ight\}$$

where the minimum is taken over all pairs (i, j), $1 \le i < j \le n$, such that the vertices i and j are adjacent.

Proof. Since $\lambda_1 = 1 - \rho_n = 1 + |\rho_n|$, the proof is immediate using the upper bound on $|\rho_n|$ given by Theorem 4. \Box

EXAMPLE 1. G:



 $b(i,j) = \frac{\left|N_{i} \cap N_{j}\right|}{\max\left\{d_{i}, d_{j}\right\}}$

For this graph

$$b(1,2) = \frac{1}{2}$$

$$b(1,3) = b(2,3) = b(3,4) = b(3,5) = \frac{1}{5}, \ b(3,6) = \frac{2}{5}$$

$$b(4,6) = b(5,6) = \frac{1}{3}.$$

Then $\min_{i \sim j} b(i, j) = \frac{1}{5}$. Hence the largest modulus of the negative Randić eigenvalues is bounded above by $\frac{4}{5}$ and the largest normalized Laplacian eigenvalue is bounded above by $\frac{9}{5} = 1.8$. To four decimal places the smallest signless Laplacian eigenvalue of \mathscr{G} is 0.7411. Since $\Delta = 5$, the upper bound in (2) becomes $2 - \frac{0.7411}{5} = 1.8518$.

Let

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