

On Harary spectral radius with given parameters

Zhongxun Zhu, Hongyun Wei, Xiaojun Ma, Tengjiao Wang,
Wenjing Zhu

College of Mathematics and Statistics, South Central University for
Nationalities,
Wuhan 430074, P.R. China

Abstract. The Harary spectral radius $\rho(G)$ of a graph G is the largest eigenvalue of the Harary matrix $RD(G)$. In this paper, we determine graphs with the largest Harary spectral radius in four classes of simple connected graphs with n vertices: with given matching number, vertex connectivity, edge connectivity and chromatic number, respectively.

Keywords: Harary matrix, matching number, vertex connectivity, chromatic number

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1. Introduction

All graphs considered in this paper are finite, undirected and simple. Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. The distance $d_{i,j}$ is defined as the length of the shortest path between v_i and v_j in G . The diameter d of a graph is the maximum distance between any two vertices of G . The Harary matrix $RD(G)$ [3] of G , is an $n \times n$ matrix $(RD_{i,j})$ such that

$$RD_{i,j} = \begin{cases} \frac{1}{d_{i,j}}, & \text{if } i \neq j, \\ 0, & \text{if } i = j. \end{cases}$$

The Harary spectral radius $\rho(G)$ of a graph G is the largest eigenvalue of the Harary matrix $RD(G)$. In [4], Ivanciuc et al. have shown that $\rho(G)$ is able to produce fair QSPR models for the boiling points, molar heat capacities, vaporization enthalpies, refractive indices and densities for $C_6 - C_{10}$ alkanes. Hence it is an interesting topic to study the maximum

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eigenvalue of $RD(G)$. Note that $RD(G)$ is a real symmetric matrix, its all eigenvalues are real. Further by the Perron-Frobenius theorem, we know that there is a unique positive eigenvector corresponding to $\rho(G)$ whose entries sum to 1 if G is connected.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [1].

Two edges of G are said to be independent if they are not adjacent in G . A set of pairwise independent edges in G is called a matching in G . A matching of maximum cardinality is a maximum matching in G . The matching number $\beta(G)$ (or just β , for short) of the graph G is the number of edges in a maximum matching. Let $\mathcal{G}_{n,\beta}$ be the set of graphs on n vertices with matching number β . Let M be an arbitrary matching in G . A path in G which starts at an unmatched vertex and then contains, alternately, edges from $E(G) \setminus M$ and from M , is an alternating path with respect to M . An alternating path P that ends at unmatched vertices is called an augmenting path.

The vertex connectivity of a graph G is the minimum number of vertices whose deletion yields a disconnected graph, and the edge connectivity of a graph G is the minimum number of edges whose deletion yields a disconnected graph. The components of a graph are its maximal connected subgraphs. Components of odd (even) order are called the odd (even) components. Denote by $\mathcal{G}_{n,\kappa}$ the set of graphs with n vertices and vertex connectivity κ , and $\mathcal{G}_{n,\kappa'}$ the set of graphs with n vertices and edge connectivity κ' .

Two vertices of G are said to be independent if they are not adjacent in G . The chromatic number of a graph G is the smallest number of colors needed to color the vertices of G such that any two adjacent vertices have different colors. A subset of vertices assigned to the same color is called a color class, every such class forms an independent set. The Turán graph $T_{n,r}$ is a complete r -partite graph on n vertices for which the number of vertices of vertex classes are as equal as possible. Let $\mathcal{C}_{n,r}$ be the set of graphs on n vertices with chromatic number r .

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs. The union $G_1 \cup G_2$ is defined to be $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. The join $G_1 \vee G_2$ of G_1 and G_2 is obtained from $G_1 \cup G_2$ by joining edges from each vertex of G_1 to each vertex of G_2 . We denote by \overline{K}_n the graph on n vertices with no edges.

Let $J_{a \times b}$ be the $a \times b$ matrix whose entries are all equal to 1 and I_n be the $n \times n$ unit matrix. For simplicity, if $a = b$, we write J_a instead of $J_{a \times a}$.

In this paper, we determine graphs with the largest Harary spectral

radius in four classes of simple connected graphs with n vertices: with given matching number, vertex connectivity, edge connectivity and chromatic number, respectively.

We list some known results which will be used in this paper.

Let $o(G)$ be the number of odd components of G .

Lemma 1.1. (The Tutte-Berge Formula)[2, 5, 7] Suppose G is a graph on n vertices with matching number β . Then there exists a subset $S_0 \subset V(G)$ on s vertices in G such that $n - 2\beta = \max\{o(G - S) - |S| : S \subset V(G)\} = o(G - S_0) - |S_0| = q - s$, where $q = o(G - S_0)$.

Lemma 1.2. [6] Let G be a connected graph with $n \geq 2$ vertices, m edges and diameter d . Then $\rho(G) \geq \frac{2m}{n} + \frac{1}{d}(n - 1 - \frac{2m}{n})$, with equality if and only if G is a complete graph K_n or G is a regular graph of diameter 2.

2. Main results

Let $v_k, v_l \in V(G)$ and $v_k v_l \notin E(G)$, adding edge $v_k v_l$ to G does not increase distance, while it does decrease at least one distance; the distance between v_k and v_l is one in $G + v_k v_l$ and at least two in G . Let $RD(G')$ be the Harary matrix of G' , then $RD(G')_{i,j} \geq RD(G)_{i,j}$ for all $v_i, v_j \in V(G)$. Moreover, $1 = RD(G')_{k,l} > RD(G)_{k,l}$, by the Perron-Frobenius theorem, we conclude that

$$\rho(RD(G')) > \rho(RD(G)) \quad (2.1)$$

Lemma 2.1. Let $G = K_s \vee (\bigcup_{i=1}^q K_{n_i})$ and

$$x(G) = (\underbrace{x_1, \dots, x_1}_{n_1}, \underbrace{x_2, \dots, x_2}_{n_2}, \dots, \underbrace{x_q, \dots, x_q}_{n_q}, \underbrace{y, \dots, y}_s)$$

be a unit eigenvector of $RD(G)$ corresponding to $\rho(G)$, if $n_q \geq n_i \geq 2, 1 \leq i \leq q - 1$, then $n_q x_q - n_i x_i + x_i > 0$.

Proof. By $RD(G)x(G) = \rho(G)x(G)$, we have

$$\begin{aligned} \rho(G)x_i &= \frac{1}{2}n_1 x_1 + \dots + \frac{1}{2}n_{i-1} x_{i-1} + (n_i - 1)x_i + \frac{1}{2}n_{i+1} x_{i+1} + \dots + \\ &\quad \frac{1}{2}n_{q-1} x_{q-1} + \frac{1}{2}n_q x_q + sy; \\ \rho(G)x_q &= \frac{1}{2}n_1 x_1 + \frac{1}{2}n_2 x_2 + \frac{1}{2}n_3 x_3 + \dots + \frac{1}{2}n_{q-1} x_{q-1} + \\ &\quad (n_q - 1)x_q + sy. \end{aligned}$$

Then

$$x_q = \frac{\rho(G) - \frac{n_i}{2} + 1}{\rho(G) - \frac{n_q}{2} + 1} x_i.$$

Hence

$$\begin{aligned} n_q x_q - n_i x_i + x_i &= \frac{\rho(G) - \frac{n_i}{2} + 1}{\rho(G) - \frac{n_q}{2} + 1} n_q x_i - n_i x_i + x_i \\ &\geq n_q x_i - n_i x_i + x_i > 0. \end{aligned}$$

□

Lemma 2.2. *Let G be a graph with maximal Harary spectral radius in $\mathcal{G}_{n,\beta}$, then there exist positive odd numbers n_1, n_2, \dots, n_q such that $G = K_s \vee (\bigcup_{i=1}^q K_{n_i})$ with $s = q + 2\beta - n$ and $\sum_{i=1}^q n_i = n - s$.*

Proof. Let M be a maximum matching in G , then $|M| = \beta$. By Lemma 1.1, there exists a subset $S_0 \subset V(G)$ on s vertices in G such that

$$n - 2\beta = \max\{o(G - S) - |S| : S \subset V(G)\} = q - s,$$

where $q = o(G - S_0)$. Let G_1, G_2, \dots, G_q be the odd components in $G - S_0$ with $|V(G_i)| = n_i \geq 1$ for $i = 1, 2, \dots, q$. Clearly, $n \geq s + q = n + 2s - 2\beta$. Thus $s \leq \beta$.

Case 1 If $s = 0$, then $G - S_0 = G$ and $n + s - 2\beta = n - 2\beta = q \leq 1$ since G is connected. If $q = 0$, then $n = 2\beta$; If $q = 1$, then $n = 2\beta + 1$. In both case, by (2.1), we have $G \cong K_n$.

Case 2 If $s \geq 1$, then $q = n + s - 2\beta \geq 1$ since $n \geq 2\beta$.

First, we claim that $G - S_0$ contains no even component.

In fact, if it doesn't hold, let W be an even component of $G - S_0$. Then by adding an edge to G between a vertex v_{i_0} of W and a vertex v_{j_0} of an odd component of $G - S_0$, we obtain a graph G' , for which

$$n - 2\beta(G') \geq o(G - S_0) - |S_0| = o(G - S_0) - |S_0| = n - 2\beta(G),$$

note that $\beta(G) \leq \beta(G')$ since $G \subset G'$. So $\beta(G) = \beta(G')$, then $G' \in \mathcal{G}_{n,\beta}$. Let D' be the Harary matrix of G' . Obviously, $RD(G)_{i,j} \leq RD(G')_{i,j}$ and $RD(G)_{i_0,j_0} < RD(G')_{i_0,j_0}$ for the new edge $v_{i_0}v_{j_0}$. Then by Perron-Frobenius theorem, we conclude that $\rho(G) < \rho(G')$, a contradiction.

Second, we claim that $G_1 \cong K_{n_1}$.

It is obvious for $n_1 = 1$, now we assume that $n_1 \geq 3$ in the following. If $G_1 \not\cong K_{n_1}$, then there exist two vertices $v_i, v_j \in V(G_1)$ with $v_i v_j \notin E(G_1)$. Then by adding the edge $v_i v_j$ to G , we obtain a graph \tilde{G} , for which

$$n - 2\beta(\tilde{G}) \geq o(\tilde{G} - S_0) - |S_0| = o(G - S_0) - |S_0| = n - 2\beta(G),$$

then $\beta(G) \geq \beta(\tilde{G})$. Further, we have $\beta(G) = \beta(\tilde{G})$ and $\rho(G) < \rho(\tilde{G})$, also a contradiction. Similarly, we have G_2, \dots, G_q , the subgraph induced by S_0 are all complete, and any vertex of G_i ($i = 1, 2, \dots, q$) is adjacent to every vertex in S_0 . So $G = K_s \vee (\bigcup_{i=1}^q K_{n_i})$. \square

Lemma 2.3. *If $n_q \geq n_i \geq 2, 1 \leq i \leq q-1$, $G = K_s \vee (\bigcup_{j=1}^q K_{n_j})$, $G' = K_s \vee (\bigcup_{j=1}^{i-1} K_{n_j} \cup K_{n_{i-1}} \cup (\bigcup_{j=i+1}^{q-1} K_{n_j}) \cup K_{n_{q+1}})$, then $\rho(G') > \rho(G)$.*

Proof. Without loss of generality, let $i = 1$, then $RD(G') =$

$$\begin{pmatrix} J_{(n_1-1)} - E_{(n_1-1)} & \cdots & \frac{1}{2}J_{(n_1-1) \times 1} & \frac{1}{2}J_{(n_1-1) \times n_q} & J_{(n_1-1) \times s} \\ \frac{1}{2}J_{n_2 \times (n_1-1)} & \cdots & \frac{1}{2}J_{n_2 \times 1} & \frac{1}{2}J_{n_2 \times n_q} & J_{n_2 \times s} \\ \cdots & & & & \\ \frac{1}{2}J_{1 \times (n_1-1)} & \cdots & 0 & J_{1 \times n_q} & J_{1 \times s} \\ \frac{1}{2}J_{n_q \times (n_1-1)} & \cdots & J_{n_q \times 1} & J_{n_q} - E_{n_q} & J_{n_q \times s} \\ J_{s \times (n_1-1)} & \cdots & J_{s \times 1} & J_{s \times n_q} & J_{s \times s} - E_s \end{pmatrix}$$

and $RD(G) =$

$$\begin{pmatrix} J_{(n_1-1)} - E_{(n_1-1)} & \cdots & J_{(n_1-1) \times 1} & \frac{1}{2}J_{(n_1-1) \times n_q} & J_{(n_1-1) \times s} \\ \frac{1}{2}J_{n_2 \times (n_1-1)} & \cdots & \frac{1}{2}J_{n_2 \times 1} & \frac{1}{2}J_{n_2 \times n_q} & J_{n_2 \times s} \\ \cdots & & & & \\ J_{1 \times (n_1-1)} & \cdots & 0 & \frac{1}{2}J_{1 \times n_q} & J_{1 \times s} \\ \frac{1}{2}J_{n_q \times (n_1-1)} & \cdots & \frac{1}{2}J_{n_q \times 1} & J_{n_q} - E_{n_q} & J_{n_q \times s} \\ J_{s \times (n_1-1)} & \cdots & J_{s \times 1} & J_{s \times n_q} & J_{s \times s} - E_s \end{pmatrix}$$

So $RD(G') - RD(G) =$

$$\begin{pmatrix} 0 & 0 & \cdots & -\frac{1}{2}J_{(n_1-1) \times 1} & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 \\ \cdots & & & & & \\ -\frac{1}{2}J_{1 \times (n_1-1)} & 0 & \cdots & 0 & \frac{1}{2}J_{1 \times n_q} & 0 \\ 0 & 0 & \cdots & \frac{1}{2}J_{n_q \times 1} & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 \end{pmatrix}$$

Let

$$x(G) = (\underbrace{x_1, \dots, x_1}_{n_1-1}, \underbrace{x_2, \dots, x_2}_{n_2}, \dots, \underbrace{x_{q-1}, \dots, x_{q-1}}_{n_{q-1}}, x_1, \underbrace{x_q, \dots, x_q}_{n_q}, \underbrace{y, \dots, y}_s)$$

be a unit eigenvector of $RD(G)$ corresponding to $\rho(G)$, then

$$x(G)(RD(G') - RD(G))x(G)^T = x_1(n_q x_q - n_1 x_1 + x_1),$$

by Lemma 2.1, we have $x_1(n_q x_q - n_1 x_1 + x_1) > 0$. So

$$\rho(G') \geq x(G)RD(G')x(G)^T > x(G)RD(G)x(G)^T = \rho(G).$$

□

Theorem 2.4. *Let $G \in \mathcal{G}_{n,\beta}$, then*

- (i) *If $n = 2\beta$ or $n = 2\beta + 1$, then $\rho(G) \leq \rho(K_n)$ with equality if and only if $G \cong K_n$;*
- (ii) *If $n \geq 2\beta + 2$, then $\rho(G) \leq \rho(K_1 \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{n-2\beta} \cup K_{2\beta-1})$ with equality if and only if $G \cong K_1 \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{n-2\beta} \cup K_{2\beta-1}$.*

Proof. (i) If $n = 2\beta$ or $n = 2\beta + 1$, by (2.1), it is easy to see $\rho(G) \leq \rho(K_n)$ and the equality holds if and only if $G \cong K_n$.

(ii) If $n \geq 2\beta + 2$, let G^* be the graph with maximal Harary spectral radius, by Lemma 2.2, we know that G^* has the form of the following: $K_s \vee (\cup_{i=1}^q K_{n_i})$ with $s = q + 2\beta - n$ and $\sum_{i=1}^q n_i = n - s$. Repeated by Lemma 2.3, we know that $G^* \cong K_s \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{q-1} \cup K_{n_q}$, where $q = n + s - 2\beta$, $n_q = 2\beta - 2s + 1$, that is, $G^* \cong K_s \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{n+s-2\beta-1} \cup K_{2\beta-2s+1}$.

Note that

$$K_s \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{n+s-2\beta-1} \cup K_{2\beta-2s+1} \subset K_{s-1} \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{n+s-2\beta-2} \cup K_{2\beta-2s+3},$$

then

$$\begin{aligned} & \rho(K_s \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{n+s-2\beta-1} \cup K_{2\beta-2s+1}) \\ & < \rho(K_{s-1} \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{n+s-2\beta-2} \cup K_{2\beta-2s+3}). \end{aligned}$$

Further we have $G^* \cong K_1 \vee \underbrace{(K_1 \cup \dots \cup K_1)}_{n-2\beta} \cup K_{2\beta-1}$. □

Theorem 2.5. *Let $G \in \mathcal{G}_{n,\kappa}$, then $\rho(G) \leq \rho(K_\kappa \vee (K_1 \cup K_{n-1-\kappa}))$ with equality if and only if $G \cong K_\kappa \vee (K_1 \cup K_{n-1-\kappa})$.*

Proof. Let G^* be the graph with maximal Harary spectral radius in $\mathcal{G}_{n,\kappa}$, by (2.1), we know that $G^* \cong K_\kappa \vee (K_{n_1} \cup K_{n_2})$ with $\kappa + n_1 + n_2 = n$ and $n_1 \leq n_2$. If $n_1 \geq 2$, let $G' = K_\kappa \vee (K_{n_1-1} \cup K_{n_2+1})$, by Lemma 2.3, we have $\rho(G') > \rho(K_\kappa \vee (K_{n_1} \cup K_{n_2}))$, a contradiction. Hence $G^* \cong K_\kappa \vee (K_1 \cup K_{n-1-\kappa})$. \square

Theorem 2.6. *Let $G \in \mathcal{G}_{n,\kappa'}$, then $\rho(G) \leq \rho(K_{\kappa'} \vee (K_1 \cup K_{n-1-\kappa'}))$ with equality if and only if $G \cong K_{\kappa'} \vee (K_1 \cup K_{n-1-\kappa'})$.*

Proof. Let G be a graph in $\mathcal{G}_{n,\kappa'}$ and κ its vertex connectivity. It is well known that $\kappa \leq \kappa'$. If $\kappa = \kappa'$, by Theorem 2.5, we have $\rho(G) \leq \rho(K_{\kappa'} \vee (K_1 \cup K_{n-1-\kappa'}))$. If $\kappa < \kappa'$, by Theorem 2.5 and (2.1), we have $\rho(G) \leq \rho(K_\kappa \vee (K_1 \cup K_{n-1-\kappa})) < \rho(K_{\kappa'} \vee (K_1 \cup K_{n-1-\kappa'}))$. \square

Theorem 2.7. *Let $G \in \mathcal{C}_{n,r}$, then $\rho(G) \leq \rho(T_{n,r})$ with equality if and only if $G \cong T_{n,r}$.*

Proof. Let G^* be the graph with maximal Harary spectral radius in $\mathcal{C}_{n,r}$, by (2.1), we know that $G^* \cong K_{n_1, n_2, \dots, n_r}$ with $n_1 + \dots + n_r = n$. If there exist $i, j \in \{1, 2, \dots, r\}$ such that $n_i - n_j \geq 2$, let

$$G' = K_{n_1, \dots, n_{i-1}, n_i-1, n_{i+1}, \dots, n_{j-1}, n_j+1, n_{j+1}, \dots, n_r}.$$

Without loss of generality, set $i = 1, j = 2$, that is, $G' = K_{n_1-1, n_2+1, n_3, \dots, n_r}$. Note that $RD(G') =$

$$\begin{pmatrix} \frac{1}{2}(J_{n_1-1} - E_{n_1-1}) & J_{(n_1-1) \times 1} & J_{(n_1-1) \times n_2} & \cdots & J_{(n_1-1) \times n_r} \\ J_{1 \times (n_1-1)} & 0 & \frac{1}{2}J_{1 \times n_2} & \cdots & J_{1 \times n_r} \\ J_{n_2 \times (n_1-1)} & \frac{1}{2}J_{n_2 \times 1} & \frac{1}{2}(J_{n_2} - E_{n_2}) & \cdots & J_{n_2 \times n_r} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ J_{n_r \times (n_1-1)} & J_{n_r \times 1} & J_{n_r \times n_2} & \cdots & \frac{1}{2}(J_{n_r} - E_{n_r}) \end{pmatrix},$$

and $RD(G) =$

$$\begin{pmatrix} \frac{1}{2}(J_{n_1-1} - E_{n_1-1}) & \frac{1}{2}J_{(n_1-1) \times 1} & J_{(n_1-1) \times n_2} & \cdots & J_{(n_1-1) \times n_r} \\ \frac{1}{2}J_{1 \times (n_1-1)} & 0 & J_{1 \times n_2} & \cdots & J_{1 \times n_r} \\ J_{n_2 \times (n_1-1)} & J_{n_2 \times 1} & \frac{1}{2}(J_{n_2} - E_{n_2}) & \cdots & J_{n_2 \times n_r} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ J_{n_r \times (n_1-1)} & J_{n_r \times 1} & J_{n_r \times n_2} & \cdots & \frac{1}{2}(J_{n_r} - E_{n_r}) \end{pmatrix},$$

then

$$RD(G') - RD(G) = \begin{pmatrix} 0 & \frac{1}{2}J_{(n_1-1) \times 1} & 0 & \cdots & 0 \\ \frac{1}{2}J_{1 \times (n_1-1)} & 0 & -\frac{1}{2}J_{1 \times n_2} & \cdots & 0 \\ 0 & -\frac{1}{2}J_{n_2 \times 1} & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

By symmetry, we can set $x(G) = (\underbrace{x_1, \dots, x_1}_{n_1}, \underbrace{x_2, \dots, x_2}_{n_2}, \dots, x_1, \underbrace{x_r, \dots, x_r}_{n_r})^T$ be a unit eigenvector of $RD(G)$ corresponding to $\rho(G)$, then $RD(G)x(G) = \rho(G)x(G)$. Hence

$$\begin{aligned} \frac{1}{2}(n_1 - 1)x_1 + n_2x_2 + n_3x_3 + \dots + n_r x_r &= \rho(G)x_1 \\ n_1x_1 + \frac{1}{2}(n_2 - 1)x_2 + n_3x_3 + \dots + n_r x_r &= \rho(G)x_2, \end{aligned}$$

then $x_2 = \frac{\rho + \frac{n_1+1}{2}}{\rho + \frac{n_2+1}{2}}x_1$. Note that

$$\begin{aligned} \rho(G') - \rho(G) &\geq x(G)^T (RD(G') - RD(G))x(G) \\ &= \frac{1}{\rho + \frac{n_2+1}{2}} [(n_1 - n_2 - 1)\rho(G) + \frac{n_1}{2} - n_2 - \frac{1}{2}]x_1^2 \\ &\geq \frac{x_1^2}{\rho + \frac{n_2+1}{2}} (\rho(G) + \frac{n_1}{2} - n_2 - \frac{1}{2}). \end{aligned}$$

By Lemma 1.2, we have

$$\begin{aligned} \rho(G) &\geq \frac{2m}{n} + \frac{1}{d}(n - 1 - \frac{2m}{n}) \\ &\geq 1 + \frac{n-1}{2} > 1 + \frac{n_1-1}{2}. \end{aligned}$$

Hence $\rho(G') - \rho(G) > \frac{x_1^2}{\rho + \frac{n_2+1}{2}}(n_1 - n_2) > 0$, a contradiction. Hence $G^* \cong T_{n,r}$. \square

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