Supporting information file for Sharp Bounds and Normalization of Wiener-type Indices

We describe here detailed proofs of Theorems 1-4. We start with some definitions and three Lemmas.

A matrix \( A = (a_{ij})_{1 \leq i,j \leq n} \) is majorized by matrix \( B = (b_{ij})_{1 \leq i,j \leq n} \), denoted by \( A \preceq B \) or \( B \succeq A \) if and only if

\[
a_{(i)} \leq b_{(i)} \quad \text{for } 1 \leq i \leq n 
\]

where \( a_{(i)} \) and \( b_{(i)} \) are the \( i \)-th smallest elements in \( A \) and \( B \). \( A \) is strictly majorized by \( B \), denoted by \( A < B \) or \( B > A \) if and only if

\[
a_{(i)} \leq b_{(i)} \quad \text{for } 1 \leq i \leq n 
\]

and

\[
a_{(i)} < b_{(i)} \quad \text{for some } i.
\]

Matrices \( A \) and \( B \) are said to be equivalent, denoted by \( A \equiv B \) if and only if

\[
a_{(i)} = b_{(i)} \quad \text{for } 1 \leq i \leq n.
\]

Majorization, strict majorization, and equivalent between two vectors \( A = (a_i)_{1 \leq i \leq n} \) and \( B = (b_i)_{1 \leq i \leq n} \) are defined similarly.

Let \( G \) be a graph, define \( V(G) \) as the set of nodes in \( G \), and \( E(G) \) as the set of edges in \( G \). Let \( \deg_G(u) \) denote the degree of node \( u \) in graph \( G \). When there is no risk of ambiguity which graph \( G \) we are considering, we abbreviate \( \deg_G(u) \) to \( \deg(u) \). Define \( ne(u) = \{ v \in V(G) : (u, v) \in E(G) \} \) and call it neighborhood of node \( u \). A node of degree 1 is called a pendant node or a leaf. A node which is not a pendant node is called an internal node.

A tree is called a starlike tree if it has exactly one node of degree greater than two. Figures 1(c), 1(f), and 1(g) show 8-node starlike trees with maximum degree equal to 5, 4, and 5 respectively.

**Lemma 1** Let \( T \) be a connected tree, \( u_1 \) a pendant node and \( u_2 \) an internal node. Suppose all nodes, if there is any, in the shortest path connecting \( u_1 \) and \( u_2 \) are of degree 2. Then

\[
(d(u_2, v))_{v \in V(T)} < (d(u_1, v))_{v \in V(T)}.
\]
**Proof.** Let $P_{u_1,u_2}$ denote the path connecting $u_1$ with $u_2$. For $v \in V(T) \setminus V(P_{u_1,u_2})$

$$d(u_1, v) = d(u_1, u_2) + d(u_2, v) > d(u_2, v).$$

And

$$d(u_1, v)_{v \in V(P_{u_1,u_2})} \equiv d(u_2, v)_{v \in V(P_{u_1,u_2})}.$$

Thus

$$(d(u_2, v))_{v \in V(T)} < (d(u_1, v))_{v \in V(T)}.$$

\(\square\)

**Lemma 2** Consider two distinct trees $T_1$ and $T_2$. Let $u_1, u_2 \in V(T_1)$ with $u_1$ of degree at least 2 and $u_2$ a pendant node satisfying the property that any node, if there is any, on the shortest path connecting $u_1$ and $u_2$ is of degree 2. Let $u_3 \in V(T_2)$. A new tree $T$ is constructed by connecting $u_1$ and $u_3$, and $T'$ is constructed by connecting $u_2$ and $u_3$. Then,

$$D(T) < D(T').$$

**Proof.** Observe that

$$(d(v_1, v_2))_{v_1,v_2 \in V(T_1)} \equiv (d'(v_1, v_2))_{v_1,v_2 \in V(T_1)};$$

$$(d(v_1, v_2))_{v_1,v_2 \in V(T_2)} \equiv (d'(v_1, v_2))_{v_1,v_2 \in V(T_2)}.$$ 

For $v_1 \in V(T_2)$, we have

$$(d'(v_1, u_3))_{v_2 \in V(T_1)} 
\equiv d'(v_1, u_3) + 1 + (d'(u_2, v_2))_{v_2 \in V(T_1)} 
\equiv d(v_1, u_3) + 1 + (d(u_2, v_2))_{v_2 \in V(T_1)}$$

and
Figure S1. Illustrating the choices of $u_1, u_2$ and $u_3$ in Lemma 2. Here $T_1$ has 5 nodes, $T_2$ 3 nodes. We choose $u_1 = 3, u_2 = 5$ and $u_3 = 6$. Tree $T$ is constructed by joining $u_1$ and $u_3$ while $T'$ by joining $u_2$ and $u_3$. $D(T)$ and $D(T')$ are $8 \times 8$ matrices where the first 5 columns correspond to the 5 nodes in $T_1$, and the last 3 rows correspond to the 3 nodes in $T_2$.

Thus $D(T) \prec D(T')$. $\square$

Manipulations in Lemma 2 are illustrated in Figure S1.

Starting from a tree $T$ with $m$ number of nodes with maximum degree $\Delta(T)$. If $m \geq 2$, Lemma 2 can be iteratively applied to construct a tree $T'$ such that the maximum degree is equal to that of $T$ but the
number of nodes in $T'$ with the maximum degree is reduced by 1. If $m = 1$, then Lemma 2 can also be iteratively applied to construct a tree $T'$ with maximum degree $\Delta(T') = \Delta(T) - 1$.

**Lemma 3** Given $i + j = k + \ell = n$, $1 \leq \ell < i < j < k$, $T$ is created by connecting internal node $u_1$ of $S_i$ and internal node $u_2$ of $S_j$. $T'$ is created by connecting internal node $u_3$ of $S_k$ and internal node $u_4$ of $S_{\ell}$. Then

$$(d'(u_3, v))_{v \in V(T')} \prec (d(u_1, v))_{v \in V(T)},$$

$$D(T') \prec D(T).$$

**Proof.** Note that $|V(T)| = |V(T')| = n$.

Note also that $(d(u_1, v))_{v \in V(T)}$ has 1 entry equals to 0, $i$ entries equal to 1 and $j - 1$ entries equal to 2. Similarly $(d'(u_3, v))_{v \in V(T')}$ has 1 entry equals to 0, $k$ entries equal to 1 and $\ell - 1$ entries equal to 2. Thus $(d(u_3, v))_{v \in V(T')} \prec (d(u_1, v))_{v \in V(T)}$ proving the first majorization.

Both $D(T)$ and $D(T')$ have $n$ entries equal to 0, $2(n - 1)$ entries equal to 1. $D(T)$ has $2(i - 1)(j - 1)$ entries equal to 3 and the rest of entries 2, $D(T')$ has $2(k - 1)(\ell - 1)$ entries equal to 3 and the rest of entries 2. Since $(k - 1)(\ell - 1) < (i - 1)(j - 1)$, thus $D(T') \prec D(T)$ proving the second majorization, and hence the proof of Lemma 3. \hfill $\square$

Manipulations in Lemma 3 are illustrated in Figure S2, where $n = 10$, $i = j = 5$, $\ell = 3$, $k = 7$.

**Proof of Theorem 2**

In this section we will find upper and lower bounds of $W_f(T)$ for $T \in \mathcal{T}_n$. Lemmas 4 and 5 are dedicated to investigate the relationship between a tree’s distance matrix and its maximum degree.

Consider the following subtree pruning and regrafting (SPR) algorithm:

**Input** $T \in \mathcal{T}_n$ with $\Delta(T) \geq 3$:

1. Choose a pendant node $u_1$, and an internal node $u_2$ with $\text{deg}(u_2) \geq 3$ satisfying the condition that all nodes lying on the shortest path connecting $u_1$ and $u_2$, if any, are of degree 2.

2. Choose $u_3 \in ne(u_2)$ such that $u_3$ does not lie on the shortest path connecting $u_1$ and $u_2$.

3. A new tree $T' \in \mathcal{T}_n$ is constructed by first deleting $(u_2, u_3)$ and then connecting $u_3$ to $u_1$.
Figure S2. Illustration of Lemma 3. Here $n = 10, i = j = 5, \ell = 3, k = 7$. From the counts of the distances above, it is clear that $(d'(u_3, v))_{v \in V(T')} < (d(u_1, v))_{v \in V(T)}$ and $D(T') \prec D(T)$.

This algorithm outputs a tree $T^0$ with these properties: (i) $D(T) \prec D(T^0)$; (ii) $\Delta(T) - 1 \leq \Delta(T^0) \leq \Delta(T)$; and (iii) number of pendant nodes is one less than that of $T$.

To see this, let $P_{u_1,u_2}$ denote the path connecting $u_1$ with $u_2$. Observe that

$$(d(v_1, v_2))_{v_1, v_2 \in V(T) \setminus V(P_{u_1,u_2})} = (d^0(v_1, v_2))_{v_1, v_2 \in V(T) \setminus V(P_{u_1,u_2})}$$

and

$$(d(v_1, v_2))_{v_1, v_2 \in V(P_{u_1,u_2})} = (d^0(v_1, v_2))_{v_1, v_2 \in V(P_{u_1,u_2})}.$$

For $v_1 \in V(T) \setminus V(P_{u_1,u_2})$, we have

$$(d(v_1, v_2))_{v_2 \in P_{u_1,u_2}} = d(v_1, u_3) + 1 + (d(u_2, v_2))_{v_2 \in P_{u_1,u_2}}$$

and
Figure S3. Illustration of the subtree pruning and regrafting algorithm. Here $T_0$ is obtained from $T$ first by deleting the edge $(u_2, u_3)$ and then connecting $u_1$ and $u_3$. $T_0$ is proved to satisfy these properties: (i) $D(T) \prec D(T^0)$; (ii) $\Delta(T) - 1 \leq \Delta(T^0) \leq \Delta(T)$; and (iii) number of pendant nodes is one less than that of $T$.

Thus $D(T) \prec D(T^0)$ and property (i) follows. Since $\deg_{T^0}(u_2) = \deg_T(u_2) - 1$, $\deg_{T^0}(u_1) = 2$, $\deg_{T^0}(u) = \deg_T(u)$ for $u \neq u_1, u_2$. Then properties (ii) and (iii) follow.

Manipulations of SPR algorithms are illustrated in Figure S3.

**Lemma 4** Let $T \in \mathcal{T}_n$ with $\Delta(T) \geq 3$. There exists $T' \in \mathcal{T}_n$ such that $\Delta(T') = \Delta(T) - 1$ and

$$D(T) \prec D(T').$$

**Proof.** Let $\ell$ be the number of pendant nodes in $T$. Apply SPR algorithm to $T$ to obtain $T^0$. If
$\Delta(T^0) = \Delta(T) - 1$, then we stop and take $T' = T^0$. Otherwise let $T = T^0$ and apply SPR algorithm again. We repeat this algorithm until we obtain the desired tree $T'$. Note that this algorithm will be repeated at most $\ell$ times to get the desired tree.

**Lemma 5** Let $T \in \mathcal{T}_n$ with $2 \leq \Delta(T) < n - 1$. There exists $T' \in \mathcal{T}_n$ such that $\Delta(T') = \Delta(T) + 1$ and $D(T') \prec D(T)$.

**Proof.** We write $\Delta(T) = k$. Choose $u \in V(T)$ with degree $m$ in such a way that all its neighbors except one are pendant nodes. Write $\text{ne}(u) = \{u_1, \ldots, u_{m-1}, u_m\}$ where $u_m$ is the only internal node in $T$. We consider two cases: 1: $m - 1 + \deg_T(u_m) < k + 1$ and 2: $m - 1 + \deg_T(u_m) \geq k + 1$.

1. A new tree $T^0$ is constructed by deleting edge $(u, u_j)$, and then connecting $u_j$ to $u_m$ for $1 \leq j \leq m - 1$. We claim that $T^0$ satisfies $\Delta(T^0) = k$ and $D(T^0) \prec D(T)$. Since $\deg_{T^0}(v) = \deg_T(v), v \in V(T) \setminus \{u, u_m\}, \deg_{T^0}(u) = 1, \deg_{T^0}(u_m) = \deg_T(u_m) + m - 1 \leq k$, so $\Delta(T^0) = k$. $D(T^0) \prec D(T)$ follows from Lemma 3. Let $T = T^0$ and repeat this procedure again. Note that the number of pendant nodes in $T$ increases by 1 for each application of this procedure.

2. A new tree $T^0$ is constructed by deleting edge $(u, u_j)$, and connecting $u_j$ to $u_m$ for $1 \leq j \leq k - \deg_T(u_m)$. As in case 1, $T^0$ satisfies $D(T^0) \prec D(T)$. Since $\deg_{T^0}(v) = \deg_T(v), v \in V(T) \setminus \{u_1, u_m\}, \deg_{T^0}(u) = \deg_T(u) - (k + 1 - \deg_T(u_m)) < k, \deg_{T^0}(u_m) = k + 1$, so $\Delta(T^0) = k + 1$. Let $T' = T^0$ and $T'$ satisfies conditions in Lemma 5.

In either case, we shall eventually produce a tree as required in Lemma 5.

Since the star graph has the largest maximum degree, and the path graph has the smallest maximum degree among trees in $\mathcal{T}_n$, by Lemmas 4 and 5, we obtain the following corollary.

**Corollary 1** Let $T \in \mathcal{T}_n$ with $2 < \Delta(T) < n - 1$. Then

$$D(S_n) \prec D(T) \prec D(P_n).$$

**Proof of Theorem 2** Applying Corollary 1 and the fact that $f$ is increasing.

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Proof of Theorem 1

Define $G_n(m)$ as a set of connected graphs with the number of nodes $n$ and the number of edges $m$.

First we will show that maximum value of $W_f(G)$ over $G \in G_n(m)$ is a monotone function of the number of edges, $m$, of $G$.

**Lemma 6** Let $G \in G_n$. Then $\max_{G \in G_n(m)} W_f(G)$ and $\min_{G \in G_n(m)} W_f(G)$ are decreasing functions in $m$.

**Proof.** For any $G \in G_n$ with $D(G) = (d(i,j))_{1 \leq i,j \leq n}$. Since $m \geq n$, $G$ cannot be a tree and hence contains a cycle. Choose an edge in a cycle in $G$ and delete it to form $G'$. Let’s say the deleted edge is $(1,2)$. Note that $G' \in G_n(m-1)$. Write $D(G') = (d'(i,j))_{1 \leq i,j \leq n}$. Since $E(G) \subset E(G')$, $d(i,j) \leq d'(i,j)$, $1 \leq i < j \leq n$, $W_f(G) \leq W_f(G')$. So $\max_{G \in G_n(m)} W_f(G) \leq \max_{G \in G_n(m-1)} W_f(G)$, for $m \geq n$.

Consider $n \leq m \leq \frac{n(n-1)}{2}$. For any $G \in G_n(m-1)$, we connect two nodes with distance greater than 1 in $G$ and call the resulting graph $G''$. Now $G'' \in G_n(m)$ with $D(G'') = (d''(i,j))_{1 \leq i,j \leq n}$. Since $E(G) \subset E(G'')$, $d''(i,j) \leq d(i,j)$, $1 \leq i < j \leq n$, thus $W_f(G'') \leq W_f(G)$. So $\min_{G \in G_n(m)} W_f(G) \leq \min_{G \in G_n(m-1)} W_f(G)$ for $m \geq n$.

**Proof of Theorem 1** From Lemma 6 we have

$$W_f(K_n) \leq W_f(G) \leq \max\{W_f(T) : T \in T_n\}.$$

From Theorem 2

$$W_f(P_n) = \max\{W_f(T) : T \in T_n\}.$$

Thus Theorem 1 follows.

**Proof of Theorem 3**

In this section, we consider trees with a given maximum degree. The relationship between the distance matrix and the number of nodes with degree equal to maximum degree is investigated.

**Lemma 7** Let $T \in T_n$ with $n_1$ nodes with degree equal to $\Delta(T)$. Suppose $n_1 \geq 2$ and $\Delta(T) \geq 3$. There exists $T' \in T_n$ with $\Delta(T') = \Delta(T)$ and $n_1 - 1$ nodes with degree equal to $\Delta(T)$. Moreover, we have

$$D(T) \prec D(T').$$
Proof. Let ℓ be the number of pendant nodes in T. Apply SPR algorithm to T to obtain T⁰. If T⁰ has n₁ − 1 nodes with degree equal to Δ(T), then we stop and take T' = T⁰. Otherwise let T = T⁰ and apply SPR algorithm again. We repeat this algorithm until we obtain desired tree T'. Note that this algorithm will be repeated at most ℓ − n₁ + 1 times to obtain desired tree.

Corollary 2 Let T ∈ Tn with 2 < Δ(T) < n − 1. There exists a starlike tree T' with Δ(T) = Δ(T') such that

\[ D(T) < D(T') \]

Corollary 2 states that among trees with equal maximum degree, distance matrix of a tree with more than one node with maximum degree is strictly majorized by a distance matrix of a starlike tree. Next to find a tree whose distance matrix majorizes all starlike trees.

Lemma 8 Let T be a starlike tree with Δ(T) = k ≥ 3. Then

\[ D(T) \preceq D(B_{n,k+1}) \]

with equality holds if and only if T is B_{n,k+1}.

Proof. Assume T is non-isomorphic to B_{n,k+1}. Denote by u the node with maximum degree k, by u₁, . . . , uₖ pendant nodes in T, and by Vᵢ set of nodes in the shortest path connecting node u and uᵢ, 1 ≤ i ≤ k. Next a new tree T⁰ is constructed by deleting edge (uₖ₋₁, ne(uₖ₋₁)) and connecting uₖ₋₁ to uₖ.

For i, j ∈ V \ {uₖ₋₁},

\[ d(i, j) = d⁰(i, j). \]

For i ∈ V \ (Vₖ₋₁ ∪ Vₖ)

\[ d(i, uₖ₋₁) = d(i, u) + d(u, uₖ₋₁) \]
\[ d⁰(i, uₖ₋₁) = d⁰(i, u) + d⁰(u, uₖ₋₁) = d(i, u) + d(u, uₖ) + 1 \]

thus
\[ d(i, u_{k-1}) < d^0(i, u_{k-1}). \]

And

\[ (d(i, u_{k-1}))_{V_{k-1} \cup V_k} = (d^0(i, u_{k-1}))_{V_{k-1} \cup V_k}, \]

since both vectors are distances of a pendant node to other nodes in one path with length \( d(u_{k-1}, u_k) \).

Thus \( D(T) \prec D(T^0) \). If \( T^0 \) satisfies \( d^0(u, u_1) = \cdots = d^0(u, u_{k-1}) = 1 \), then we stop and \( T^0 \) is \( B_{n,k+1} \). Otherwise let \( T = T^0 \) and we repeat this process until get tree \( B_{n,k+1} \). Note that this algorithm will be repeated \( n - k - d(u, u_k) \) times. \( \square \)

**Lemma 9** For \( k \geq 3 \),

\[ D(B_{n,k+1}) \prec D(B_{n,k}) \]

**Proof.** Lemma 9 follows directly from Lemmas 4 and 8. \( \square \)

**Proof of Theorem 3** Applying Lemma 8 and the fact that \( f \) is increasing.

**Remark** It has been proven in corollary 3.5 of [1] that

\[ W_f(T_n(k)) = \min \{ W_f(T) : T \in \mathcal{T}_n, \Delta(T) = k \} \quad (\ast) \]

where \( T_n(k) \) is a \( k \)-ary tree, also called Volkmann tree [2]. It remains open whether

\[ D(T_n(k)) \preceq D(T) \quad \text{for } T \in \mathcal{T}_n, \Delta(T) = k \quad (\ast\ast) \]

holds for all \( k, n \) and \( k \leq n \). We have verified that \( (\ast\ast) \) holds for \( 6 \leq n \leq 9 \) and \( k = 3 \). If \( (\ast\ast) \) is true for all \( n \) and \( k \), it provides an alternative proof of

\[ W_f(T_n(k)) \leq W_f(T) \]

for \( T \in \mathcal{T}_n, \Delta(T) = k \), and \( f \) monotonically increasing.
Proof of Theorem 4

Proof. Let $T$ be a spanning tree of $G$ satisfying $\Delta(T) = k$. Similar to the proof of Theorem 1, one can prove that $D(G) \preceq D(T)$. By Theorem 3, $D(T) \preceq D(B_{n,k+1})$. Thus $W_f(G) \leq W_f(B_{n,k+1}). \square$

References
