Faster Treewidth-based Approximations for Wiener Index

Giovanna K Conrado, Amir K Goharshady, Pavel Hudec, Pingjiang Li, Harshit J Motwani

Faster Treewidth-based Approximations for Wiener Index

Giovanna Kobus Conrado
Amir Kafshdar Goharshady
Pavel Hudec
Pingjiang Li
Harshit Jitendra Motwani
Department of Computer Science and Engineering
Department of Mathematics
Hong Kong University of Science and Technology (HKUST)
Clear Water Bay, Hong Kong, China

Abstract

The Wiener index of a graph G is the sum of distances between all pairs of its vertices. It is a widely used graph property in chemistry, initially introduced to examine the link between boiling points and structural properties of alkanes, which later found notable applications in drug design. Thus, computing or approximating the Wiener index of molecular graphs, i.e. graphs in which every vertex models an atom of a molecule and every edge models a bond, is of significant interest to the computational chemistry community.

In this work, we build upon the observation that molecular graphs are sparse and tree-like and focus on developing efficient algorithms parameterized by treewidth to approximate the Wiener index. We present a new randomized approximation algorithm using a combination of tree decompositions and centroid decompositions. Our algorithm approximates the Wiener index within any desired multiplicative factor $(1+\epsilon)$ in time $O(n \cdot \log n \cdot k^3 + \sqrt{n} \cdot k/\epsilon^2)$, where n is the number of vertices of the graph and k is the treewidth. This time bound is almost-linear in n.

Finally, we provide experimental results over standard benchmark molecules from PubChem and the Protein Data Bank, showcasing the applicability and scalability of our approach on real-world chemical graphs and comparing it with previous methods.

2012 ACM Subject Classification Applied computing → Chemistry; Theory of computation → Graph algorithms analysis; Theory of computation → Data structures design and analysis

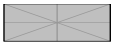
Keywords and phrases Computational Chemistry, Treewidth, Wiener Index

Digital Object Identifier 10.4230/LIPIcs.CVIT.2016.23

1 Introduction

Motivation. The Wiener index of a graph G is the sum of the distances between all pairs of vertices in G. Besides being a natural problem to compute, it is also a well-studied graph invariant with applications in computational chemistry and biology. Indeed, it is one of computational chemistry's oldest and most important topological indices [37].

History. In chemistry, the Wiener index was first considered by Harry Wiener in [40]. It was initially studied to establish connections between alkanes' boiling points and the underlying graphs' structural properties. This study later motivated the development of other topological indices in computational chemistry. Further development of QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) models led to the discovery of positive correlations of even more chemical and physical properties to the Wiener index [28, 37, 38, 42]. Due to its simplicity and usefulness, the Wiener index was also studied by computer scientists and mathematicians [16, 35]. The use



of neural networks in chemical graph theory has led to a renewed interest in topological indices and their application in molecular mining, toxicity detection, and computer-aided drug discovery. Several studies have been conducted on this topic, such as [5, 15, 17, 24, 41]. Given the significance of the Wiener index for chemists and the abundance of large molecules, it is imperative to develop faster algorithms for computing it. Indeed, there are many previous works in this direction [7, 9, 14, 21, 29].

Parameterized Algorithms. Parameterized algorithms aim to tackle computationally intractable problems and identify subsets of instances that can be solved efficiently [11]. In parameterized complexity, we consider an additional parameter k along with the input size n for measuring the runtime. This is in contrast to classical complexity theory, which only considers the input size of the problem. Many parameterized algorithms focus on NP-hard problems and provide runtime bounds that depend polynomially on the size of the problem but have non-polynomial dependence on the parameter k. If we know that k is small in real-world instances, this leads to solutions that are effectively polynomial-time, i.e. they take polynomial time on all the real-world instances where this parameter is small.

Fixed-Parameter Tractable (FPT). Given an input of size n and a parameter k, an algorithm with a running time of $O(f(k) \cdot n^c)$, for some constant c and computable function f, is called *Fixed-Parameter Tractable (FPT)* [11]. The intuition is the same as above. If the parameter k is small in all real-world instances of the problem, then the algorithm would in practice have a polynomial runtime. Crucially, the degree c of this polynomial does not depend on either k or n.

Treewidth. Treewidth is one of the most important structural parameters of graphs and has been extensively studied in combinatorics and graph theory. Intuitively speaking, it measures the tree-likeness of a graph [4]. Trees and forests have a treewidth of 1 and cliques on n vertices have treewidth $n-1$. The main advantage of treewidth in algorithm design arises when we are designing parameterized algorithms for NP-hard problems by considering it as the parameter of the problem. Many families of commonly-studied graphs, such as trees, cacti, series-parallel graphs, outer-planar graphs, and control-flow graphs of structured programs, have bounded treewidth [2, 4, 11]. This allows efficient dynamic programming techniques using the tree decomposition of the graph [2]. See Section 2 for a formal definition.

Treewidth of Molecules. Extending this idea, computational chemists and biologists have also explored the treewidth of various important classes of molecules [43, 45]. In our experimental results (Section 4), we observe that a significant majority of molecules in the PubChem repository [19] have a treewidth of at most 10. Even large proteins from the Protein Data Bank [32] are observed to have a treewidth of at most 5. Since a significant fraction of molecules have bounded treewidth, exploring and designing treewidth-based parameterized algorithms for computational problems in chemistry and biology is a natural step. In fact, the same has been done in several works in the literature [1, 7, 10, 39, 44]. We extend this line of research by presenting significantly faster treewidth-based approaches for approximating the Wiener index.

Our Contribution. In this paper, we introduce a novel randomized algorithm that approximates the Wiener index of a graph using its tree decomposition. The unique aspect of our algorithm is the incorporation of tree and centroid decompositions. This idea significantly enhances efficiency in answering distance queries within the graph. This is then plugged directly into an established randomized algorithm to approximate the Wiener index, obtaining the same approximation guarantees by an asymptotically faster method. Both theoretical analysis and experimental results demonstrate that our algorithm

Table 1 Comparison of Different Algorithms for Computing the Wiener Index. Here, n denotes the number of vertices, k denotes the treewidth, and ϵ represents the error of approximation.

Algorithm	Time Complexity	Type	Ref.
Floyd-Warshall	$O(n^3)$	Exact	[18]
Orthogonal Range Searching	$O(n \cdot \log^{k-1} n)$	Exact Parameterized	[7]
Treewidth-based Dynamic Programming	$O(n^2 \cdot k^2)$	Exact Parameterized	[8]
BFS	$O(n^2 \cdot k)$	Exact Parameterized	[30, 46]
Classical Approximation	$O(n^{5/2}/\epsilon^2)$	Randomized Approximation	[21]
Our Algorithm	$O(n \cdot \log n \cdot k^3 + \sqrt{n} \cdot k/\epsilon^2)$	Parameterized Randomized Approximation	Sec. 3

outperforms current methods in calculating the Wiener index for molecular graphs, which are commonly encountered in computational chemistry and biology.

Comparison with Previous Results. Table 1 compares the runtime complexity of our algorithm with previous methods. Here, n is the number of vertices in the graph, k is the treewidth, and ϵ is the error in the approximation, i.e. we are reporting the runtime for a $(1+\epsilon)$-approximation of the Wiener index. We refer to Section 4 for a detailed experimental evaluation of our algorithm on datasets from PubChem [19] and the Protein Data Bank [32].

The most classical approach to compute the Wiener index is simply performing an all-pairs shortest path computation using Floyd-Warshall and then summing up the distances. This will lead to a time complexity of $O(n^3)$. In [7], the authors provided the first parameterized algorithm for the Wiener index based on treewidth. Their algorithm is a divide-and-conquer method based on orthogonal range searching and repeatedly finds small cuts using the tree decomposition. They achieve a runtime bound of $O(n \cdot \log^{k-1} n)$. Note that this is not FPT. In [8], an FPT algorithm was provided based on dynamic programming on the tree decomposition. This algorithm has a quadratic dependence on n. For unweighted graphs, given that a graph with treewidth k has $O(n \cdot k)$ vertices, running a BFS from each vertex would lead to a total runtime of $O(n^2 \cdot k)$. Finally, [21] provides an algorithm on general graphs, not using any parameters, that approximates the average pairwise distance within a factor of $(1+\epsilon)$ with a probability of at least 2/3 by taking a random sample of the distances between pairs of vertices. Note that the Wiener index is n^2 times the average distance. Thus, this algorithm is directly applicable to our setting, as well. Our algorithm builds upon the classical approximation of [21] and uses a tree decomposition and a centroid decomposition to speed up the sampling.

2 Preliminaries

In this section, we introduce the Wiener index and define some basic concepts of parameterized complexity. We refer to [11] for more details. This is followed by a short presentation of the classical approximation algorithm of [21], which forms the basis of our approach.

Wiener Index [40]. The Wiener Index of an undirected graph $G = (V, E)$ is defined as the all-pairs sum of distances among vertices of the graph. Formally,

$$W(G) := \sum_{u,v \in V} d(u, v).$$

Additionally, we define the average distance between pairs of vertices in G as $\overline{d}(G) := W(G)/n^2$.

▶ Remark 1. In this work we assume that our graphs are connected, unweighted, and undirected. In the context of molecular graphs, all types of covalent bonds—be they single, double, or triple—are represented as a single undirected edge in the corresponding graph. For a disconnected graph, the Wiener index is simply $+\infty$. However, in some applications, the Wiener index of a disconnected graph is defined as the sum of the Wiener indices of its connected components. In such cases, each connected component can be processed separately.

Tree Decomposition (TD) [23, 33, 34]. A *tree decomposition* of a given graph $G = (V, E_G)$ is a tree $T = (\mathcal{B}, E_T)$ satisfying the following conditions:

- Every node $b \in \mathcal{B}$ of T, which is called a *bag,* contains a subset of vertices $V_b \subseteq V$.
- The bags cover the entire vertex set V of G, i.e. $\bigcup_{b\in\mathcal{B}} V_b = V$. In other words, every vertex appears in at least one bag.
- For every edge in the original graph G, there exists a bag that contains both endpoints of the edge. More formally, for every $e = \{u, v\} \in E_G$, there is a bag $b \in \mathcal{B}$, s.t. $u, v \in V_b$.
- Every vertex $v \in V$ appears in a connected subtree of T, meaning that the set $\mathcal{B}_v = \{b \in \mathcal{B} \mid v \in V_b\}$ forms a connected subgraph of T.

▶ Remark 2. An equivalent statement of the last condition above is that for every three bags $b_1, b_2, b_3 \in \mathcal{B}$, if b_3 is on the unique path from b_1 to b_2 in T, then $V_{b_1} \cap V_{b_2} \subseteq V_{b_3}$.

Treewidth [33]. The *width* of a tree decomposition T is defined as $w(T) := \max_{b\in\mathcal{B}} |V_b| - 1$, i.e. the size of the largest bag minus one. Furthermore, the *treewidth* of the graph G, denoted as $\mathrm{tw}(G)$, is defined as the minimum width amongst all possible tree decompositions of G.

Intuitively speaking, treewidth measures the structural likeness of a graph to a tree. Specifically, the smaller the treewidth of a graph, the more tree-like it appears, in the sense that a graph of treewidth k can be decomposed into small parts (bags), each of size at most $k + 1$, which are connected to each other in a tree-like manner T. Figure 1 showcases an illustration containing two distinct tree decompositions of a graph G, each having a different width. Since only forests have treewidth of 1, the tree decomposition on the right is optimal, and $\mathrm{tw}(G) = 2$.

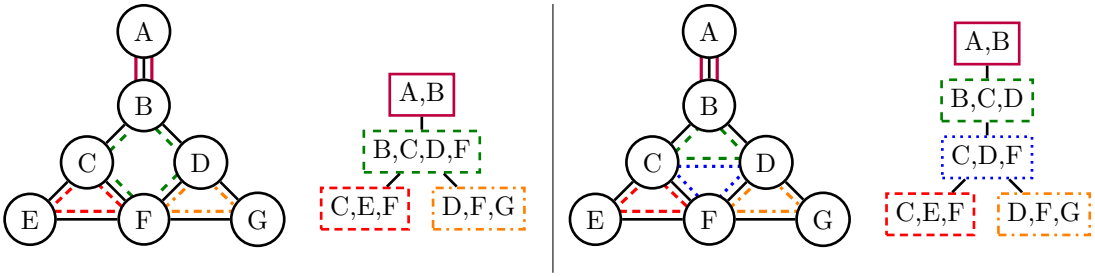


Figure 1 A Graph G and Two Tree Decompositions of G of Width 3 (left) and 2 (right).

Treewidth is a parameter indicating graph sparsity, providing an upper bound on the number of edges. Specifically, in a graph with n vertices and treewidth k, the number of edges is $O(n \cdot k)$. More precisely, the number of edges is less than or equal to $n \cdot k - k \cdot (k + 1/2)$ [31]. Additionally, we have the following ubiquitous lemma:

▶ **Lemma 3** (Cut Lemma [11]). *Let $T = (\mathcal{B}, E_T)$ be a tree decomposition of $G = (V, E_G)$. Consider two vertices $u, v \in V$ and two arbitrary bags $b_u, b_v \in \mathcal{B}$ such that $u \in b_u$ and $v \in b_v$. If*

$b \in \mathcal{B}$ is a bag on the unique path from b_u to b_v in T, then any path from u to v in G will intersect V_b. Additionally, if $e = \{b_1, b_2\} \in E_T$ is an edge on the unique path from b_u to b_v in T, then any path from u to v in G will intersect $V_{b_1} \cap V_{b_2}$.

Computing Tree Decompositions. It is well-known that the treewidth of a graph, as well as an optimal tree decomposition with $O(n)$ bags, can be computed by a linear-time FPT algorithm (parameterized by the treewidth itself) [3]. Additionally, there are many well-optimized tools for this task. Thus, in the sequel, we assume without loss of generality that an optimal tree decomposition of our graph is given as a part of the input.

Centroid [25]. Consider a tree $T = (V_T, E_T)$ with n vertices. We define a *centroid node* of T as a node whose removal breaks the tree down into several subtrees such that no resulting subtree has a size greater than $n/2$. In other words, a centroid is a $1/2$ separator of T. It is well-known that every tree has at least one centroid node, which can be obtained in linear time by dynamic programming.

Centroid Decomposition (CD) [6, 12]. A *centroid decomposition* of T is another tree T' on the same set of vertices as T, recursively defined as follows:

- When $|V_T| = 1$, we simply have $T' = T$.
- For a more complex tree, we first identify a centroid node r of T, then position this node as the root of T'.
- Once we have selected a centroid node r and removed it from T, we end up separating the original tree into several connected subtrees. Let us denote these as $T_1, T_2, \ldots, T_m$. For each subtree T_i, we find a centroid decomposition T_i' with a root r_i. We make each r_i a child of r.

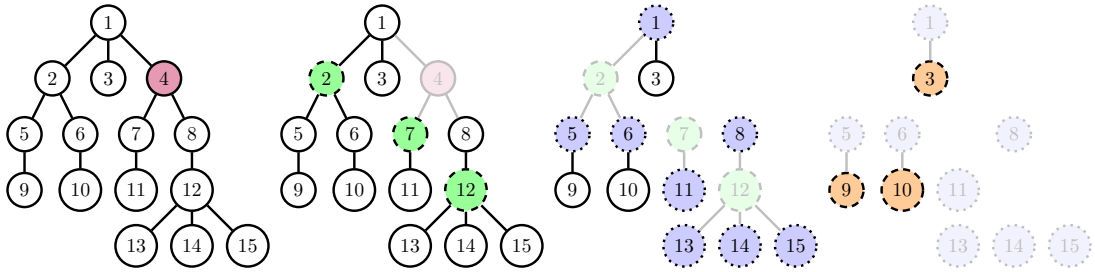


Figure 2 A Graph G and the Steps of Building its Centroid Decomposition. Each step highlights the centroid vertex of each of the current components of the graph.

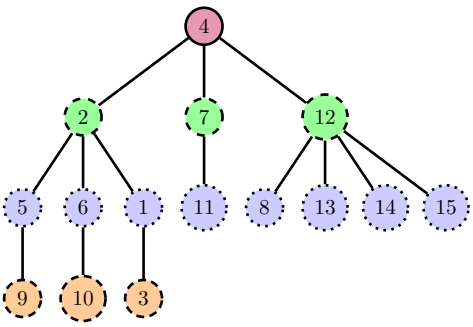


Figure 3 The Resulting Centroid Decomposition of G.

Figure 2 shows the steps of computing a centroid decomposition. Each color corresponds to a distinct layer of the centroid decomposition, with the node representing the centroid of the similarly colored dotted subtree. In this illustration, the node 4 is identified as the centroid of the initial tree. Following the removal of node 4, nodes $2, 7$, and 12 are selected as the centroids of each resulting subtree. Subsequent centroids are determined in a recursive manner. The final centroid decomposition is shown in Figure 3.

Properties of CDs. The height of a CD is bounded by $O(\log n)$, where n is the number of vertices in the original tree. This is because, with every new layer added to the centroid decomposition, each connected component splits into several parts, each no larger than $1/2$ the size of the original component. Consequently, we can append at most $O(\log n)$ layers to the centroid decomposition. Additionally, CDs satisfy the following useful lemma:

▶ **Lemma 4** (Proof in Appendix A). *Let $u, v \in V_T$ be two vertices of the original tree T and l be their lowest common ancestor in the centroid decomposition T'. The unique path connecting u and v in T must visit l.*

Computing Centroid Decompositions. Given a tree T with n vertices, there are a variety of algorithms in the literature that compute a centroid decomposition T' of T in $O(n)$. Examples include [6, 12].

Lowest Common Ancestor Queries. Consider a rooted tree T with n vertices. Suppose we have q offline queries, each providing two vertices $u, v \in T$ and asking for their lowest common ancestor. The classical algorithm of Gabow and Tarjan [20] solves this problem and answers all queries in $O(n + q)$.

Approximation Algorithm of [21]. The work [21] provides an elegant and simple approximation algorithm for the average distance $\overline{d}(G)$ between pairs of vertices. Since the Wiener index is simply $n^2 \cdot \overline{d}(G)$, the same algorithm can be reused for our problem. Given a graph G and an error bound ϵ as the input, the algorithm in [21] works as follows:

1. Uniformly select $\Theta(\sqrt{n}/\epsilon^2)$ pairs of vertices.
2. Find the distance between each selected pair of vertices.
3. Output the average of the computed distances.

Surprisingly, this algorithm provides a $(1+\epsilon)$-approximation of $\overline{d}(G)$ with probability $2/3$.

▶ **Theorem 5** ([21], Theorem 5.1). *Given G and ϵ as input, the algorithm above outputs a $(1+\epsilon)$-approximation of $\overline{d}(G)$ with probability at least $2/3$.*

As a direct corollary, a $(1+\epsilon)$-approximation of the Wiener index can be computed in the same time complexity by simply multiplying the result of this algorithm by n^2.

Complexity Analysis. For general graphs, each distance query can take $O(n^2)$ time. Thus, the total runtime of the algorithm above is $O(n^{5/2}/\epsilon^2)$. However, if the underlying graph G is guaranteed to have small treewidth k, then it can have at most $O(n \cdot k)$ vertices. Thus, each distance query can be answered in $O(n \cdot k)$ by a BFS. This reduces the runtime to $O(n^{3/2} \cdot k/\epsilon^2)$.

In this work, we build upon this simple randomized algorithm and use the treewidth to obtain a faster algorithm for distance queries. This allows us to reduce the runtime dependence on n to almost-linear.

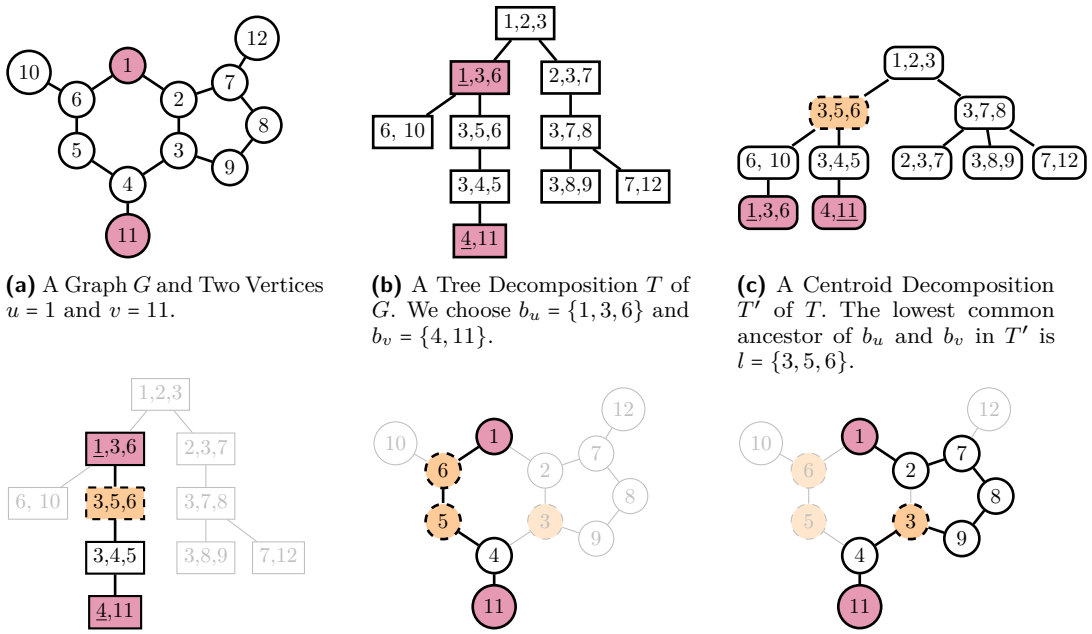
3 Our Algorithm

In this section, we present our treewidth-based algorithm. Our algorithm follows the same steps as the approximation algorithm of [21], except that we exploit the tree decomposition

to perform distance queries faster. Our main novel idea is to look not only at a tree decomposition of the underlying graph but also at a centroid decomposition of this tree decomposition. Thus, our algorithm exploits the desirable properties of both types of decomposition, as formalized by the lemma below:

▶ **Lemma 6.** *Let $G = (V, E_G)$ be a graph, $T = (\mathcal{B}, E_T)$ a tree decomposition of G and $T' = (\mathcal{B}, E_{T'})$ a centroid decomposition of T. Consider two vertices $u, v \in V$ and arbitrary bags $b_u, b_v \in \mathcal{B}$ such that $u \in b_u$ and $v \in b_v$. Let l be the lowest common ancestor of b_u and b_v in the centroid decomposition T'. Any path that goes from u to v in G intersects V_l.*

Proof. Consider the path π_T from b_u to b_v in the tree decomposition T. By Lemma 4, we have $l \in \pi_T$. By Lemma 3, any bag in π_T intersects every path from u to v in G. This is illustrated in Figure 4. ◀



(a) A Graph G and Two Vertices $u = 1$ and $v = 11$.

(b) A Tree Decomposition T of G. We choose $b_u = \{1, 3, 6\}$ and $b_v = \{4, 11\}$.

(c) A Centroid Decomposition T' of T. The lowest common ancestor of b_u and b_v in T' is $l = \{3, 5, 6\}$.

(d) The path from b_u to b_v in T goes through l.

(e) Every path from u to v in G must intersect V_l.

(f) Every path from u to v in G must intersect V_l.

Figure 4 An Illustration of Lemma 6.

Based on the lemma above, if we precompute the distances from each vertex appearing in a bag l of the centroid decomposition T' to the vertices appearing in descendants of l in T', then we can answer distance queries in $O(k)$. In other words, to find the distance from u to v, we first find two bags b_u and b_v containing them, then compute $l = \text{lca}(b_u, b_v)$. Now, we know that every path from u to v has to go through l, thus

$$d_G(u, v) = \min_{w \in V_l} \left(d_G(u, w) + d_G(w, v) \right).$$

Here, d_G denotes the distance in graph G.

Our Algorithm for Wiener Index. Based on the discussion above, given $\epsilon > 0$, a graph $G = (V, E_G)$ and a tree decomposition $T = (\mathcal{B}, E_T)$ of G with width k, our algorithm turns G into a weighted graph and takes the following steps:

- ***Step 1 (Centroid Decomposition).*** Compute a centroid decomposition T' of the tree decomposition T.
- ***Step 2 (Local Precomputation).*** For every two vertices $u, v \in V$, if there is a bag $b \in \mathcal{B}$ that contains both of them, i.e. $u, v \in V_b$, then compute the distance $d_G(u, v)$ and add a direct edge with weight $d_G(u, v)$ between u and v.
- ***Step 3 (Ancestor-Descendant Precomputation).*** Let $b_1, b_2 \in \mathcal{B}$ be two bags such that b_1 is an ancestor of b_2 in the centroid decomposition T'. For every $u \in V_{b_1}$ and $v \in V_{b_2}$, compute the distance $d_G(u, v)$ and add a direct edge with weight $d_G(u, v)$ between u and v.
- ***Step 4 (Sampling).*** Uniformly select $\Theta(\sqrt{n}/\epsilon^2)$ pairs of vertices of G as in the algorithm of [21].
- ***Step 5 (Distance Queries).*** For each pair of vertices $(u, v) \in V^2$ selected in the previous step, compute $d_G(u, v)$.
- ***Step 6 (Output).*** Output the average of all the distances obtained in the previous step.

For Step 1, we can rely on previous algorithms that compute centroid decompositions, such as [6, 12]. Steps 4 and 6 are straightforward. We now provide details of Steps 2, 3, and 5, followed by correctness proofs and runtime analyses.

Details of Step 2. This step is inspired by [8]. Given the graph $G = (V, E_G)$ and its tree decomposition $T = (\mathcal{B}, E_T)$, our goal is to create shortcut edges between any pair of vertices that appear in the same bag. We provide a recursive procedure as follows:

i. Choose a leaf bag ℓ of the tree decomposition T.
ii. Perform an all-pairs shortest-path algorithm, such as Floyd-Warshall, in $G[V_\ell]$, i.e. only on the vertices and edges in ℓ. If a path of length d is found between u and v, add a direct $\{u, v\}$ edge with weight d to G.
iii. Let $T^* = T - \ell$ and $G^* = G - \{v \in V_\ell \mid \nexists\, b \in \mathcal{B} \;\; b \neq \ell \wedge v \in V_b\}$. In other words, we are removing the leaf bag ℓ from our tree decomposition and also removing any vertex that appeared only in this bag from the graph G.
iv. Run the algorithm recursively on (G^*, T^*). This causes more shortcut edges to be added in G.
v. Repeat Step ii, i.e. perform another all-pairs shortest-path in $G[V_\ell]$ and add the resulting shortcut edges to G.

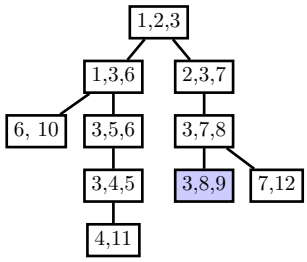
Figure 5 provides an example of this step.

▶ **Lemma 7** (Proof in Appendix B). *The procedure above runs in time $O(n \cdot k^3)$. After its execution, T is still a valid tree decomposition of G, and for every pair of vertices $u, v \in V$, if there exists a bag $b \in \mathcal{B}$ containing both of them, then there is a direct (shortcut) edge from u to v with weight $d_G(u, v)$.*

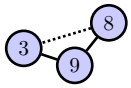
▶ Remark 8. Throughout our algorithm, we always keep at most one edge, i.e. the edge with minimum weight, between every pair $\{u, v\}$ of vertices.

Details of Step 3. In this step, we process our centroid decomposition T' in a bottom-up manner. For every bag $b \in \mathcal{B}$, we consider the subtree T'_b of the centroid decomposition T', consisting of b and all of its descendants in T'. Let G_b be the induced subgraph of G that contains all the vertices in T'_b, i.e.

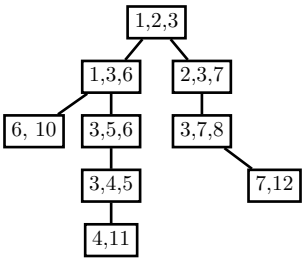
$$G_b = G\left[\bigcup_{b' \in T'_b} V_{b'}\right].$$



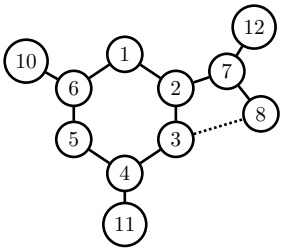
(a) We choose the leaf bag $\ell = \{3, 8, 9\}$.



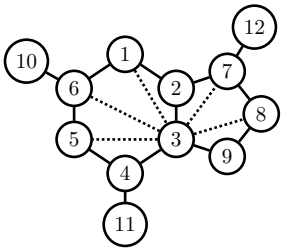
(b) Shortest paths are found within $G[V_\ell]$. Dashed lines represent newly added edges.



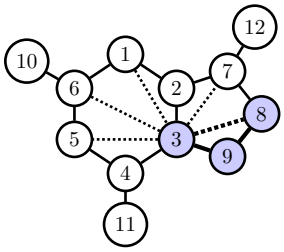
(c) Bag ℓ is removed from T to form T^*.



(d) G^* is formed by removing vertex 9 from G, since it only appears in bag ℓ in T.



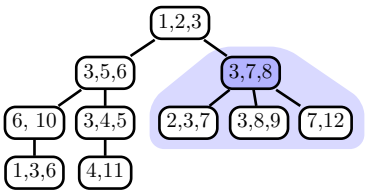
(e) After recursively running the algorithm on (G^*, T^*), new edges are added to G.



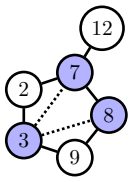
(f) Shortest paths are again found within $G[V_\ell]$ and any new edges found are added to G. In this example, no new edges were found.

Figure 5 An Example of Step 2 on the Graph and Decomposition of Figure 4.

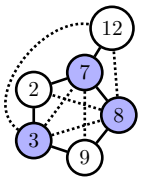
For every vertex $v \in V_b$ that appears in the bag b, our algorithm runs a shortest-path computation, such as Dijkstra's algorithm [13], from b in the graph G_b and finds its distances to all other vertices of G_b, adding the corresponding shortcut edges. See Figure 6 for an example.



(a) Let $b = \{3, 7, 8\}$. The subtree T'_b of T' is highlighted.



(b) The figure above shows G_b. We now run Dijkstra's algorithm from vertices in $\{3, 7, 8\}$.



(c) After running Dijkstra's algorithm in G_b, we add the new shortcut edges picutred above to G.

Figure 6 An Example of Step 3 on the Graph and Decompositions of Figure 4.

▶ **Lemma 9.** *The procedure above runs in $O(n \cdot \log n \cdot k^3)$. After its execution, for every two bags $b_1, b_2 \in \mathcal{B}$ such that b_1 is an ancestor of b_2 in the centroid decomposition T' and every two vertices $u \in V_{b_1}$ and $v \in V_{b_2}$, we have a shortcut edge from u to v with weight $d_G(u, v)$.*

Proof. Let α_b and δ_b be the number of ancestors and descendants of b in T', respectively. The graph G_b has $O(\delta_b \cdot k)$ vertices and thus $O(\delta_b \cdot k^2)$ edges. Moreover, we perform $O(k)$

Dijkstras* over this graph, one for each vertex in the bag b. Thus, our total runtime is

$$\sum_{b\in\mathcal{B}} O(\delta_b \cdot k^3) = \sum_{b\in\mathcal{B}} O(\alpha_b \cdot k^3) = O(n \cdot \log n \cdot k^3).$$

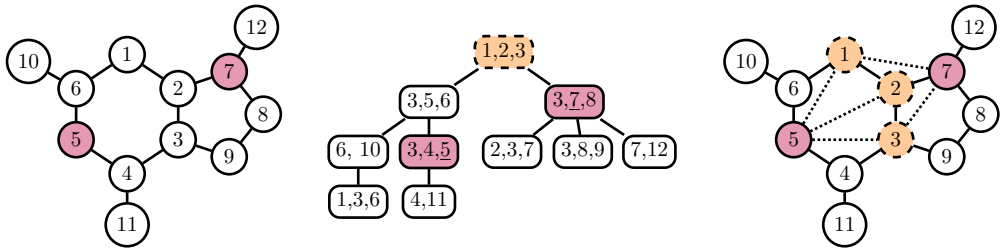
The latter equality is because every vertex has $O(\log n)$ ancestors.

For the second part, consider a shortest path π from u to v in G. Let π_T be the path from b_1 to b_2 in the tree decomposition T. By Lemma 3, π intersects the vertices of every bag b in π_T. Without loss of generality, we can assume that π stays in these bags, i.e. it only visits vertices in $\bigcup_{b\in\pi_T} V_b$. Note that if π leaves π_T, then it has to reenter it, but the exit and entry vertices are in the same bag and, by Lemma 7, there is already a shortcut edge between them. Additionally, since b_1 is an ancestor of b_2 in the centroid decomposition T', there was a point in the construction of T' when b_1 was chosen as the centroid of a connected component containing b_2. Thus, all the bags in π_T were also in the same connected component. Hence, every b is a descendant of b_1. Therefore, the entire path π is included in G_b and the Dijkstra from u finds the shortest path to v and adds the corresponding shortcut edge. ◀

Details of Step 5. Suppose our goal is to compute $d_G(u, v)$. We first pick two bags b_u and b_v such that $u \in b_u$ and $v \in b_v$. We then find the lowest common ancestor $l = \text{lca}(b_u, b_v)$. By Lemma 4, every path from u to v has to intersect V_l. Thus, we compute

$$d_G(u, v) = \min_{w\in V_l} \left(d_G(u, w) + d_G(w, v)\right).$$

Note that since l is an ancestor of both b_u and b_v, we have the distances needed on the RHS as weights of direct shortcut edges. This is illustrated in Figure 7



(a) Let $u = 5$ and $v = 7$.

(b) We select $b_u = \{3, 4, 5\}$ and $b_v = \{3, 7, 8\}$. Their lowest common ancestor l in T' is $\{1, 2, 3\}$, thus any shortest path from 5 to 7 has to go through vertices 1, 2, or 3.

(c) Since l is an ancestor of b_u and b_v, the vertices u and v have shortcut edges to every vertex in l.

Figure 7 An Example of Step 5 on the Graph and Decompositions of Figure 4.

▶ **Lemma 10.** *The procedure above returns the correct distances in* $O(n + k \cdot \sqrt{n}/\epsilon^2)$.

Proof. Correctness is already argued above. Since the centroid decomposition T' has $O(n)$ bags, preprocessing and answering offline lowest common ancestor queries takes $O(n + \sqrt{n}/\epsilon^2)$ [20]. For each of the $\sqrt{n}/\epsilon^2$ queries generated in Step 4, we should compute the minimum of $O(k)$ values since $|V_l| \le k + 1$. ◀

*Our graph is weighted at this point, but all edge weights and distances are non-negative integers less than n. Thus, Dijkstra runs in linear time on the number of vertices and edges. Intuitively, instead of keeping a priority queue of vertices in our Dijkstra, we can simply keep an array $A[n]$ of lists where $A[i]$ contains all vertices of distance i to the source.

Finally, the following is our main theorem in this work:

▶ **Theorem 11.** *Given an $\epsilon > 0$, an undirected unweighted graph $G = (V, E_G)$ with n vertices and a tree decomposition $T = (\mathcal{B}, E_T)$ of G with $O(n)$ bags and width k, our algorithm runs in time $O(n \cdot \log n \cdot k^3 + \sqrt{n} \cdot k/\epsilon^2)$ and produces a $(1+\epsilon)$-approximation of the Wiener index $W(G)$ with probability at least 2/3.*

Proof. Correctness of the approximation ratio and success probability follows from Theorem 5 since our algorithm is the same as [21] except for how we answer distance queries. Step 1 takes $O(n)$ using well-known algorithms such as [6, 12]. Step 2 takes $O(n \cdot k^3)$ based on Lemma 7. Step 3 takes $O(n \cdot \log n \cdot k^3)$ as shown in Lemma 9. Step 4 simply takes $O(\sqrt{n}/\epsilon^2)$ samples from the uniform distribution and Step 5 takes $O(n + k \cdot \sqrt{n}/\epsilon^2)$ time as per Lemma 10. Finally, Step 6 takes $O(\sqrt{n}/\epsilon^2)$ time. Summing these up leads to the desired asymptotic time complexity. ◀

4 Experimental Results

In this section, we present our experimental results, comparing the runtimes of our algorithm with previous approaches. We implemented the main algorithms in C++ and provided the same inputs, i.e. graph G, tree decomposition T and $\epsilon = 0.1$ to all of them. To obtain this input, we first used pysmiles [26], RDKit [27] and NetworkX [22] for preprocessing molecular data and turning them into graphs. We also used FlowCutter [36] to compute tree decompositions. All our experiments were conducted on an Intel Core i5 (2.3 GHz, Quad-core) Machine with 8 GB of RAM running MacOS. We enforced a time limit of 1000 seconds per instance.

Benchmarks. We used the following datasets for our experiments: (i) PubChem [19] and (ii) Protein Data Bank (PDB). Specifically, we report results on 100 randomly-selected protein molecules from the PDB database and 1,311,229 molecules from PubChem.

PDB. The Protein Data Bank (PDB) [32] is an extensive repository of three-dimensional structural data for large biological molecules, including proteins, DNA and RNA. We randomly selected 100 protein molecules from this database. Table 2 shows some statistics about these molecules. We observed that even the large molecules in this dataset have small treewidth.

Table 2 Statistics of the PDB Benchmarks

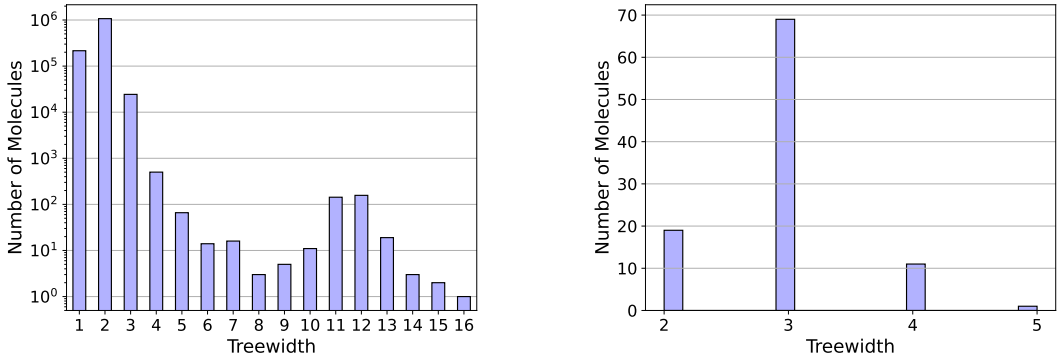
	Minimum	Maximum	Average
Number of Vertices	682	80652	9027
Number of Edges	743	82055	9240
Treewidth	2	5	2.95

PubChem. PubChem [19] is an open chemistry database of the National Institutes of Health (NIH). It includes information on chemical structures, identifiers, chemical and physical properties, and biological activities of small molecules. As benchmarks, we took the following datasets from PubChem: `Common Chemistry CAS`, `Nature Catalysis`, `Wikipedia`, `Nature Communications`, `Wiley`, `Springer Nature`, `Nature Chemistry`, `Nature Portfolio Journals`, `Springer Materials`, `Drug and Medication`, `Nature Synthesis`, `Nature Chemical Biology`, `KEGG`, `DrugBank`. Collectively, these datasets contained 1,311,229 molecules at the time of writing. See Table 3 for the statistics over this set of benchmarks.

Table 3 Statistics of the PubChem Benchmarks

Metric	Minimum	Maximum	Average
Number of Vertices	2	568	21
Number of Edges	1	643	22
Treewidth	1	16	1.8

Treewidth of the Molecules. As mentioned in Tables 2 and 3, we observed that the chemical compounds in both benchmark suites exhibit bounded treewidth. Figure 8 provides a histogram for each benchmark suite. Notably, the vast majority of PubChem compounds have a treewidth of less than 10, with very few molecules having treewidths of up to 16. In addition, the large protein molecules in the PDB dataset also have bounded treewidths of at most 5.



(a) PubChem (y-axis is in logarithmic scale) **(b)** PDB

Figure 8 Treewidth Distribution in Our Benchmarks

Results. Figure 9 compares the performance of our algorithm and previous methods over the PDB dataset, whereas Table 4 provides the same comparison for PubChem. Our approach's better asymptotic complexity leads to significant gains in efficiency when considering the large graphs in PDB. However, no benefit is observed over the PubChem molecules, since they are all small and every algorithm can handle them in under 1 ms.

Table 4 Runtime Comparison of the Algorithms of Table 1 over PubChem Benchmarks. All times are in milliseconds.

Algorithm	Maximum	Minimum	Average
Our Algorithm	1.425	0.187	0.296454
Approximation Algorithm	1.283	0.203	0.297342
DP on Tree Decomposition	1.256	0.192	0.296152
Floyd-Warshall	2.261	0.199	0.288638
Orthogonal Range Searching	1.121	0.199	0.292404
BFS	1.097	0.205	0.290523

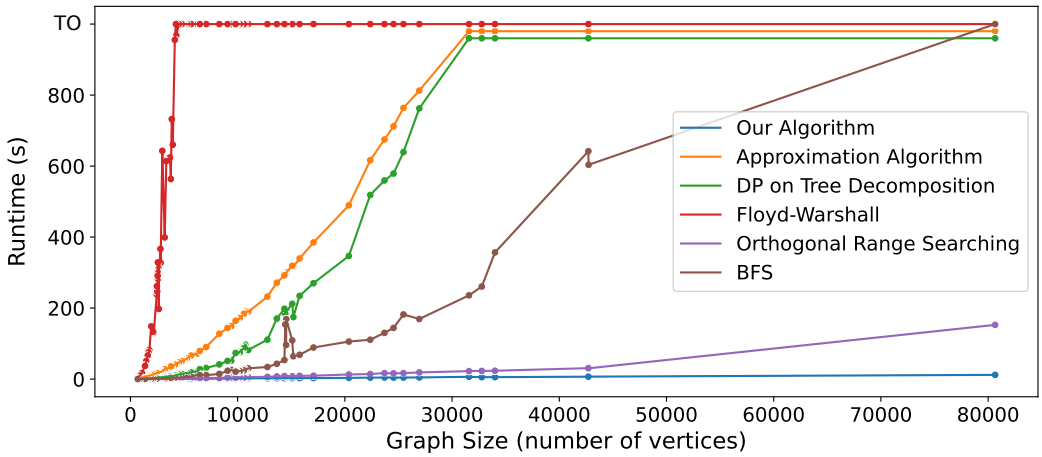


Figure 9 Runtime Comparison of the Algorithms of Table 1 over PDB Benchmarks. Each dot corresponds to one benchmark molecule.

5 Conclusion

In this work, we considered the problem of computing the Wiener index of a graph with n vertices and treewidth k. We provided a novel algorithm using a combination of tree decompositions and centroid decompositions, which achieves an almost-linear FPT runtime of $O(n \cdot \log n \cdot k^3 + \sqrt{n} \cdot k/\epsilon^2)$ and outputs a $(1+\epsilon)$-approximation of the Wiener index with probability at least 2/3. To the best of our knowledge, this is the first sub-quadratic time FPT algorithm for this problem. We also showed that many real-world molecular graphs have small treewidth and thus our algorithm is applicable in practice.

6 Acknowledgments

The research was partially supported by the Hong Kong Research Grants Council ECS Project Number 26208122.

References

1. Tatsuya Akutsu and Hiroshi Nagamochi. Comparison and enumeration of chemical graphs. *Computational and structural biotechnology journal*, 5(6):e201302004, 2013.
2. Hans L. Bodlaender. Dynamic programming on graphs with bounded treewidth. In *ICALP*, volume 317, pages 105–118, 1988.
3. Hans L. Bodlaender. A linear-time algorithm for finding tree-decompositions of small treewidth. *SIAM J. Comput.*, 25(6):1305–1317, 1996.
4. Hans L Bodlaender et al. A tourist guide through treewidth. 1992.
5. Danail Bonchev. *Chemical graph theory: introduction and fundamentals*, volume 1. CRC Press, 1991.
6. Gerth Stølting Brodal, Rolf Fagerberg, Christian N. S. Pedersen, and Anna Östlin. The complexity of constructing evolutionary trees using experiments. In *ICALP*, volume 2076, pages 140–151, 2001.
7. Sergio Cabello and Christian Knauer. Algorithms for graphs of bounded treewidth via orthogonal range searching. *Computational Geometry*, 42(9):815–824, 2009.
8. Shiva Chaudhuri and Christos D Zaroliagis. Shortest paths in digraphs of small treewidth. part i: Sequential algorithms. *Algorithmica*, 27:212–226, 2000.
9. Victor Chepoi and Sandi Klavžar. The wiener index and the szeged index of benzenoid systems in linear time. *Journal of chemical information and computer sciences*, 37(4):752–755, 1997.
10. Giovanna K Conrado, Amir K Goharshady, Harshit J Motwani, and Sergei Novozhilov. Parameterized algorithms for topological indices in chemistry. *arXiv preprint arXiv:2303.13279*, 2023.
11. Marek Cygan, Fedor V Fomin, Łukasz Kowalik, Daniel Lokshtanov, Dániel Marx, Marcin Pilipczuk, Michał Pilipczuk, and Saket Saurabh. *Parameterized algorithms*. Springer, 2015.
12. Davide della Giustina, Nicola Prezza, and Rossano Venturini. A new linear-time algorithm for centroid decomposition. In *SPIRE*, pages 274–282, 2019.
13. E Dijkstra. A note on two problems in connexion with graphs. *Numerische Mathematik*, 1:269–271, 1959.
14. Andrey A Dobrynin, Ivan Gutman, Sandi Klavžar, and Petra Žigert. Wiener index of hexagonal systems. *Acta Applicandae Mathematica*, 72:247–294, 2002.
15. Alexander G Dossetter, Edward J Griffen, and Andrew G Leach. Matched molecular pair analysis in drug discovery. *Drug Discovery Today*, 18(15-16):724–731, 2013.
16. Roger C Entringer, Douglas E Jackson, and DA Snyder. Distance in graphs. *Czechoslovak Mathematical Journal*, 26(2):283–296, 1976.
17. Ernesto Estrada and Eugenio Uriarte. Recent advances on the role of topological indices in drug discovery research. *Current Medicinal Chemistry*, 8(13):1573–1588, 2001.
18. Robert W Floyd. Algorithm 97: shortest path. *Communications of the ACM*, 5(6):345, 1962.
19. National Center for Biotechnology Information. Pubchem database. `https://pubchem.ncbi.nlm.nih.gov`.
20. Harold N. Gabow and Robert Endre Tarjan. A linear-time algorithm for a special case of disjoint set union. In *STOC*, pages 246–251, 1983.
21. Oded Goldreich and Dana Ron. Approximating average parameters of graphs. *Random Structures & Algorithms*, 32(4):473–493, 2008.
22. Aric Hagberg, Pieter Swart, and Daniel S Chult. Exploring network structure, dynamics, and function using networkx. Technical report, Los Alamos National Lab.(LANL), Los Alamos, NM (United States), 2008.
23. Rudolf Halin. S-functions for graphs. *Journal of geometry*, 8:171–186, 1976.
24. Christoph Helma. *Predictive toxicology*. CRC Press, 2005.
25. Camille Jordan. Sur les assemblages de lignes. *Journal für die reine und angewandte Mathematik*, 70:185–190, 1869.
26. Peter C Kroon. pysmiles: A python library for parsing smiles strings. `https://pypi.org/project/pysmiles/`.

27 Gregory Landrum. Rdkit: Open-source cheminformatics. `https://www.rdkit.org`.

28 Jerzy Leszczynski. *Handbook of computational chemistry*, volume 3. Springer Science & Business Media, 2012.

29 Bojan Mohar and Tomaž Pisanski. How to compute the wiener index of a graph. *Journal of mathematical chemistry*, 2(3):267–277, 1988.

30 Edward F Moore. The shortest path through a maze. In *Proc. of the International Symposium on the Theory of Switching*, pages 285–292, 1959.

31 Jaroslav Nešetřil and Patrice Ossona De Mendez. Structural properties of sparse graphs. In *Building Bridges: Between Mathematics and Computer Science*, pages 369–426. Springer, 2008.

32 RCSB. Protein data bank. `https://www.rcsb.org`.

33 Neil Robertson and Paul D Seymour. Graph minors. iii. planar tree-width. *Journal of Combinatorial Theory, Series B*, 36(1):49–64, 1984.

34 Neil Robertson and Paul D. Seymour. Graph minors. ii. algorithmic aspects of tree-width. *Journal of algorithms*, 7(3):309–322, 1986.

35 L'ubomír Šoltés. Transmission in graphs: a bound and vertex removing. *Mathematica Slovaca*, 41(1):11–16, 1991.

36 Ben Strasser and KIT algorithms group. Flowcutter: Software for computing flow-based balanced graph cuts. `https://github.com/kit-algo/flow-cutter-pace17`.

37 Nenad Trinajstic. *Chemical graph theory*. Routledge, 2018.

38 Stephan Wagner and Hua Wang. *Introduction to chemical graph theory*. CRC Press, 2018.

39 Pengfei Wan, Jianhua Tu, Shenggui Zhang, and Binlong Li. Computing the numbers of independent sets and matchings of all sizes for graphs with bounded treewidth. *Applied Mathematics and Computation*, 332:42–47, 2018.

40 Harry Wiener. Structural determination of paraffin boiling points. *Journal of the American chemical society*, 69(1):17–20, 1947.

41 Jun Xu and Arnold Hagler. Chemoinformatics and drug discovery. *Molecules*, 7(8):566–600, 2002.

42 Ling Xue and Jurgen Bajorath. Molecular descriptors in chemoinformatics, computational combinatorial chemistry, and virtual screening. *Combinatorial chemistry & high throughput screening*, 3(5):363–372, 2000.

43 Atsuko Yamaguchi, Kiyoko F Aoki, and Hiroshi Mamitsuka. Graph complexity of chemical compounds in biological pathways. *Genome Informatics*, 14:376–377, 2003.

44 Atsuko Yamaguchi, Kiyoko F Aoki, and Hiroshi Mamitsuka. Finding the maximum common subgraph of a partial k-tree and a graph with a polynomially bounded number of spanning trees. *Information Processing Letters*, 92(2):57–63, 2004.

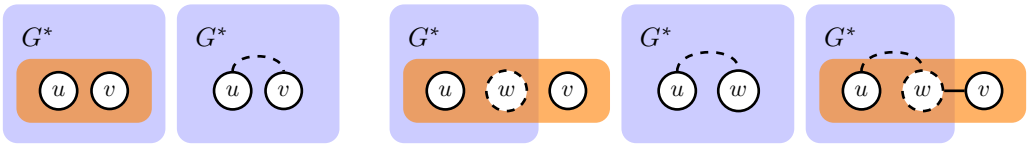
45 Atsuko Yamaguchi and Kiyoko F Aoki-Kinoshita. Chemical compound complexity in biological pathways. *Quantitative Graph Theory: Mathematical Foundations and Applications*, page 471, 2014.

46 Konrad Zuse. Der plankalkül. 1972.

A Proof of Lemma 4

Proof. We prove this lemma through induction on the size n of the tree. If n is at most 3, the lemma holds trivially. Now assume that the lemma holds for all trees with a size less than n. Let us consider a general tree of size n. In the first step, we identify a centroid node of T, denoted as c. The node c fragments T into several connected components. If any arbitrary vertices $u, v \in V_T$ exist in the same connected component T_i, then in the corresponding centroid decomposition T', they will appear in T'_i as per the definition of centroid decomposition. According to the inductive hypothesis, their path must cross their lowest common ancestor in T'_i. In case they belong to different connected components, say T'_i and T'_j, any path originating from T'_i and terminating at T'_j must traverse the node c. This is because c separates T_i and T_j. In this scenario, their lowest common ancestor would be the root c, as the remaining nodes on the path from u to v are either in T_i or T_j and, hence, cannot serve as the common ancestor. ◀

B Proof of Lemma 7



(a) When u and v appear in G^*, a shortcut edge will be calculated during the recursive call on G^*.

(b) If v is not in G^*, its path to u must contain a vertex w that is in the same bag ℓ as u and v and that also appears in G^*. A shortcut edge from u to w will be added during the processing of G^* and thus the path from u to v can be calculated in Step v.

Figure 10 An Illustration of Lemma 7.

Proof. We run the Floyd-Warshall algorithm twice on each bag of the tree decomposition, once in Step ii and once in v. Since each bag has $k+1$ vertices and the tree decomposition has $O(n)$ bags, the total runtime is $O(n \cdot k^3)$. The procedure above adds new shortcut edges only between pairs of vertices that were already in the same bag, thus the tree decomposition remains valid.

We prove the last property by induction on $|\mathcal{B}|$. If $|\mathcal{B}| = 1$, then the first Floyd-Warshall in Step ii adds all the necessary shortcut edges. Otherwise, let $u, v \in V_\ell$ be two vertices that appear in the leaf bag ℓ and let $p \in \mathcal{B}$ be the parent of ℓ in T. If there is a path between u and v that is entirely within V_ℓ, then Step ii adds a shortcut edge summarizing this path. Thus, if $u', v' \in G^*$, then $d_{G^*}(u, v) = d_G(u, v)$. Moreover, both u and v have to appear in p, since they each appear in a connected subtree. Hence, by induction hypothesis, the recursive call in Step iv adds the required shortcut edge between u and v. Now consider the case where either u or v (or both) are not in G^*. Take a shortest path π from u to v in G. If π is entirely within V_ℓ, then Step ii adds the shortcut edge. Otherwise, we use Lemma 3 to break π down as $\pi = \pi_1 \cdot w_1 \cdots w_2 \cdot \pi_2$ where π_1 is the longest prefix of π that only contains vertices from $V_\ell \setminus V_p$ and π_2 is the longest such suffix. By Lemma 3, we have $w_1, w_2 \in V_\ell \cap V_p$. Since they are both in $V_p \subseteq V_{G^*}$, Step iv adds a shortcut edge from w_1 to w_2. Hence, Step v adds a shortcut edge from u to v with the correct weight. Finally, if u and v are vertices that appear in the same bag $b \neq \ell$, then the recursive call on (G^*, T^*) adds a shortcut edge between them. ◀