

Quantifying Hierarchical Indicators of Water Distribution Network

Structure and Identifying their Relationships with Surrogate Indicators of Hydraulic Performance

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ABSTRACT

Enhancing the performance of water distribution networks (WDN) on a day-to-day basis, or under extreme disturbances is an utmost priority for utilities. Previous research has characterized the structure of WDN in the pipe-junction or segment-valve representation to gain insight on various aspects of their performance; however, the research on characterizing WDN structure in a hierarchical representation and its relationship with performance is lacking. Two key properties of WDNs are loops and pipe diameters that are organized in a hierarchical way. Novel indicators have been created to quantify the network hierarchy related to these key properties in other spatial flow distribution networks: loop nestedness and pipe diameter gradation along flow paths. The goal of this study is to adopt such indicators to characterize the hierarchy of WDNs and evaluate its relationship with WDN performance. This study applies a hierarchical decomposition process to model the relationships among loops as a tree network for quantifying loop nestedness. Flow paths of monotonically increasing and decreasing pipe diameters are traced to quantify pipe diameter gradation. Statistical distributions are approximated for these two indicators. Then, relationships between these network hierarchy indicators and two performance indicators (measuring path redundancy and power surplus) are identified. For 15 benchmark networks, this study finds the statistical

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21 distributions representing loop nestedness and pipe diameter gradation closely follow a power-law.
22 Results suggest gradual pipe diameter gradation along flow paths and high loop nestedness increase
23 WDN path redundancy, and gradual pipe diameter gradation increases WDN power surplus. The
24 study demonstrates that the hierarchical analysis of WDNs can significantly supplement traditional
25 topological analyses in explaining WDN performance.

26 **Keywords:** water distribution networks, complex network analysis, systems analysis, redundancy,
27 hierarchy

28 INTRODUCTION

29 Water distribution networks (WDNs) are lifelines of the global urban fabric. They transport
30 water to end users via a network of pipes, valves, pumps and water sources. At the same time,
31 to maintain their performance, water distribution networks face increasing stress (e.g., climate
32 related extreme weather, dwindling budgets, increased demand, aging) (ASCE, 2017; Di Nardo
33 et al., 2017; Evans et al., 2018; Gheisi et al., 2016; Blaha and Gaewski, 2007; Diao et al., 2016;
34 Butler et al., 2017; Abdel-Mottaleb et al., 2019; Pagani et al., 2020; Giustolisi, 2020). WDN
35 performance is defined as the extent to which amount, pressure, and quality of delivered water
36 are met under various scenarios (e.g., power outages, flooding) (Gheisi et al., 2016; Dziedzic and
37 Karney, 2015; Skipworth, 2002; Farmani and Butler, 2014; Pagano et al., 2019; Ostfeld et al.,
38 2002) and can be measured for both the component-level and network-wide level (Diao et al., 2016;
39 Pagano et al., 2019). Network-wide indicators of performance are useful to utilities, especially
40 in comparing design scenarios and identifying failure scenarios that cause the greatest loss in
41 service (Diao et al., 2016; Pagano et al., 2019). Thus, many indicators have and continue to be
42 defined, aiming to evaluate network-wide performance, such as reliability, resilience, robustness,
43 redundancy, and flexibility. Among them, reliability is a widely used aggregate indicator and can
44 be quantified using the probabilities of component failure, probabilities of demand exceedance,
45 and system redundancies inherent in the WDN layout— all of which can be obtained from network
46 analysis, hydraulic simulations, and/or real monitoring data (Goulter, 1987; Walski, 1987; Ostfeld
47 et al., 2002; Farmani et al., 2005; Giustolisi, 2020). Because probabilities of failure and demand

48 exceedance are not easily available (Ostfeld, 2005), entropy and the Todini index are two commonly
49 used surrogate indicators for reliability (Farmani et al., 2005; Raad et al., 2010; Reca et al., 2008;
50 Dziedzic and Karney, 2014; Ulusoy et al., 2018; Santonastaso et al., 2018). Entropy is a measure
51 of flow path redundancy. The Todini index is a measure of power surplus (which has also been
52 referred to as energy redundancy in the literature, see Ulusoy et al. (2018)). Entropy and the
53 Todini index are just two of many available reliability performance indicators (Farmani et al., 2005;
54 Ulusoy et al., 2018). Despite their limitations at capturing the totality of water distribution network
55 performance or being indirectly related to reliability, the literature has generally found that as these
56 two indicators increase, so does the reliability of a water distribution network and that the two
57 indicators each capture different aspects of WDN performance (they are by no means a complete
58 representation of hydraulic reliability or performance in general) (Farmani et al., 2005; Raad et al.,
59 2010; Reca et al., 2008; Dziedzic and Karney, 2014; Liu et al., 2017a).

60 Various factors impact the performance of WDN: internal factors such as WDN structure and
61 water hammer, and external factors such as natural disturbances and limited resources (Pagano
62 et al., 2019; Abdel-Mottaleb and Zhang, 2019). WDN structure refers to the configuration of
63 components-how they relate to each other. WDN structure can be represented in various ways,
64 including pipe-junction topology, segment-valve topology, hydraulic (or logical), and hierarchical.
65 Pipe-junction topology is what is represented by most distribution network models for hydraulic
66 simulations, where nodes represent junctions and edges represent pipes (i.e., the actual connections
67 in space). Segment-valve topology represents segments as nodes and valves as edges (Zischg
68 et al., 2017, 2019; Walski, 1993, 1994). Abdel-Mottaleb et al. (2019) and Abdel-Mottaleb and
69 Zhang (2019) investigated the so-called logical structure where nodes represent WDN components
70 (i.e., pipes, junctions) and edges represent the logical (hydraulic) influence the components have
71 on each other. The various representations of WDN structure are often analyzed via network
72 science techniques (or graph theory). The application of graph theory in WDN has been centered
73 around pipe-junction topology including characterization, connectivity analyses, sectorization, and
74 attempts to derive surrogate performance indicators (Jacobs and Goulter, 1988; Ostfeld, 2005;

75 Yazdani and Jeffrey, 2011, 2012; Ormsbee and Kessler, 1990; Hernandez et al., 2016; Giustolisi
76 et al., 2017; Giudicianni et al., 2018; Giustolisi et al., 2019; Herrera et al., 2016; Meng et al., 2018;
77 Pagano et al., 2019; Giudicianni et al., 2020; Balekelayi and Tesfamariam, 2019; Torres et al.,
78 2017) with a focus on quantifying network connectivity (Giustolisi, 2020). Though pipe-junction
79 topology is useful for hydraulic simulation and correlates with hydraulic behavior (Giustolisi,
80 2020; Walski, 1993), characterization of structure other than the pipe-junction representation is
81 also important to provide insights on WDN performance.

82 Given that water distribution systems are looped to reduce dissipation and create alternate
83 flow paths in case of breaks (Dziedzic and Karney, 2014), there is a need to consider loops in
84 network structure analysis. Previous research has developed or adopted measures considering
85 loops in a WDN, such as the ratio between numbers of existing to maximal loops in a pipe-junction
86 representation (Yazdani and Jeffrey, 2012). Such measures, however, do not distinguish between
87 "layouts with the same number of loops", and account for the organization of the loops (Singh
88 and Fiorentino, 1992). Hernandez et al. (2016) attempted to distinguish WDN layout based on
89 loops and classified WDNs as branched, grid or loopy, yet it remains qualitative and does not
90 distinguish between two different branch, grid or loopy networks. Previous research has also
91 considered pipe diameters in analyzing pipe-junction topology, such as evaluating the uniformity
92 of diameters of pipes meeting at junctions or along the loops of WDNs (Prasad and Park, 2004;
93 Creaco et al., 2016). While providing insight, the uniformity of pipe diameters along individual
94 loops or junctions does not provide a holistic network-wide characterization because it does not
95 trace flow paths in their entirety. These measures (e.g., number of loops, uniformity of pipe
96 diameters along loops) fail to represent the organization of loops and pipe diameters (i.e., how
97 the loops and pipe diameters in a WDN are arranged and organized) (Katifori and Magnasco,
98 2012; Barthelemy, 2018). The organization of both loops and pipe diameters along flow paths
99 has been represented hierarchically for many spatial flow distribution networks. Mathematically
100 representing and subsequently quantifying the hierarchy, in particular of loops and pipe diameters,
101 is a gap in the WDN literature that this study addresses. This study introduces loop nestedness and

102 pipe diameter gradation along flow paths to characterize the hierarchical representation of network
103 structure. Loop nestedness captures how loops are arranged relative to each other (e.g., which
104 smaller loops are contained within larger loops, how the number of loops changes with loop size).
105 Pipe diameter gradation along paths quantifies how gradually or abruptly diameters change along
106 the flow paths of a WDN.

107 Much less research has been conducted to relate WDN structure to performance indicators
108 than to apply network theory to characterize network structure. Studies relating WDN structure
109 to various performance indicators are skewed towards pipe-junction topology (Torres et al., 2017;
110 Meng et al., 2018; Ulusoy et al., 2018; Giustolisi et al., 2019; Giudicianni et al., 2020; Pagano
111 et al., 2019; Balekelayi and Tesfamariam, 2019). Torres et al. (2017) and Pagano et al. (2019)
112 found that though network analysis of pipe-junction topology provides insight on global WDN
113 behavior and complements physics-based hydraulic simulation, it is severely limited in explaining
114 hydraulic performance impacted by other factors. Limitations such as representing water sources in
115 the same manner as demand nodes are identified as a drawback to relating pipe-junction topology
116 to performance-based indicators (Meng et al., 2018; Giustolisi et al., 2019). Though segment-valve
117 topology accounts for water sources, the information obtained is focused on valve placement rather
118 than pipe layout (Liu et al., 2017b; Giustolisi et al., 2019; Abdel-Mottaleb and Walski, 2020).
119 As the hierarchical representation of WDNs has not yet been thoroughly characterized, there is
120 not a single study relating hierarchical measures of WDNs to hydraulic performance indicators.
121 However, the hierarchical representations of other spatial flow distribution networks have been
122 characterized and shown to provide additional insights beyond traditional connectivity/topology
123 measures, such as classification (e.g., distinguishing between different species) and correlation with
124 the redundancy and robustness to damage. (Papadopoulos et al., 2018; Ronellenfitsch and Katifori,
125 2017; Gavrilchenko and Katifori, 2018).

126 Building on previous research applying graph theory to WDNs and the research analyzing the
127 hierarchy of spatial flow distribution networks, this study proposes a methodology for characterizing
128 and quantifying hierarchy of loops and pipe diameters in WDNs. This study also evaluates how the

129 two studied hierarchical indicators, loop nestedness and pipe diameter gradation along flow paths,
130 relate to two commonly used surrogate indicators of performance based on hydraulic simulations.

131 METHODOLOGY

132 The hierarchy of spatial flow distribution networks from various domains has been characterized
133 using loop nestedness and edge diameter gradation along paths. These two indicators are quantified
134 by delineating the hierarchy, of both loops and edges (e.g., how smaller loops or edges are connected
135 to larger ones). In each domain for which these indicators have been quantified, edges represent a
136 different component (e.g., blood vessels, plant leaf veins). In this study, edge diameter refers to pipe
137 diameter. Pipe diameter gradation is measured along entire flow paths. Loop nestedness is obtained
138 after constructing a decomposition tree where nodes represent loops. If a loop is directly contained
139 in a larger loop, nodes representing the two loops are connected by an edge. After quantifying
140 and characterizing the hierarchy of WDNs, loop nestedness and pipe diameter gradation along
141 flow paths are put into physical context of the WDNs. Then, their respective contribution to water
142 distribution network performance is evaluated.

143 Benchmark water distribution networks are tested for illustration and reproducibility. The
144 networks span a large parameter space, from small number of nodes and edges, to large numbers
145 of nodes and edges; from low values of cyclicity or loops to high cyclicity values; and single
146 to multiple sources and/or pumps. Similar to [Santonastaso et al. \(2018\)](#), the networks span the
147 space of low entropy and Todini index values to high values of entropy and Todini index, and both
148 synthetic and real WDN. The WDN are analyzed in their junction-pipe layout as opposed to the
149 segment-valve representation that has been shown to be more realistic regarding isolation ([Walski,](#)
150 [1993, 1994; Liu et al., 2017b](#)). Figures of the tested WDNs and a table summarizing their properties
151 are included in the supplementary information.

152 Decomposition Process

153 This study adopts the hierarchical loop decomposition algorithm presented in [Katifori and](#)
154 [Magnasco \(2012\)](#) to obtain a decomposition tree, representing the hierarchy of loops in the network.
155 The decomposition tree is the network model used to represent hierarchical organization of loops

(i.e., representing loops contained within loops). This algorithm is part of the *nesting* python package (Ronellenfitsch et al., 2015). Prior to inputting the WDN model for decomposition, *networkx* and *WNTR*, open source python packages, are used to convert the *.inp* file for each network into a *networkx* graph object. The algorithm begins with the pruning of all nodes connected to a single edge in the water network (i.e., all junctions connected to a single pipe), only the part of the network with all edges (i.e., pipes) participating in loops remains. Then, the pipes are ordered based on their diameter, and the pipe with the smallest diameter is identified. In Figure 1, the pipe with the smallest diameter is *e1*. If there are pipes with the same diameter, the values are randomly perturbed infinitesimally such that they are no longer the same (a procedure that was found not to impact the results). Then the pipe with the smallest diameter is removed from the network. When the pipe is part of two loops, its removal leads to the merging of the two loops into a single larger loop. In Figure 1, when *e1* is removed, loops 3 and 4 merge into loop 2. The ordering of pipes and merging of loops is repeated iteratively until every pipe is removed from the network and all the loops have been merged into the largest, or most exterior, loop of the network. In Figure 1, after *e2* is removed loops 2 and 5 merge, and loop 1 is identified as the largest, most exterior loop.

In Figure 1, the resulting tree contains a single subtree. Terminal nodes of the tree are defined as the nodes for which there is no subtree; in Figure 1, the terminal nodes correspond to Nodes 5, 4, and 3. That means loops 5, 4, and 3 in the original network do not contain other loops. The subtree degree of a node is determined by the total number of terminal nodes contained in that subtree. Node 1 in Figure 2 contains three terminal nodes, and thus has a subtree degree of 3. Likewise, Node 2 contains two terminal nodes: Nodes 3 and 4. By definition, the subtree degree of terminal nodes is 0 as terminal nodes do not contain subtrees. The Nesting python package (Ronellenfitsch et al., 2015) is used to construct the decomposition tree and calculate measures representing properties of the tree. A limitation of using this algorithm is that it only allows for planar graphs (i.e pipes intersect only at their endpoints) as input. WDNs are often near-planar (Barthelemy, 2018) and the WDNs in this study are all planar.

182 **Quantification of Hierarchy: Loops**

183 *Meshedness using Pipe-Junction Representation*

184 One of the reasons we seek to quantify loop hierarchy, is to investigate how much more it can
185 explain an often-used performance indicator (entropy) of water distribution networks in comparison
186 with the commonly used measure of loops, meshedness. Meshedness has been shown to be a good
187 indicator of water distribution network redundancy (Yazdani and Jeffrey, 2011) because it is the
188 ratio of the existing number of loops to the maximal potential number of loops for the same number
189 of junctions while maintaining planarity. Meshedness (for planar networks) is calculated using the
190 following equation for the tested water distribution networks:

191
$$r = \frac{m - n + 1}{2n - 5} \quad (1)$$

192 Where m is the number of edges (i.e., pipes), and n is the number of nodes (i.e., junctions).

193 *Nestedness using Decomposed Tree*

194 Then, the water distribution networks are analyzed for their loop hierarchy using the tree network
195 from the decomposition process. Only the part of the network with the highest number of connected
196 loops is represented by the decomposition tree. If a water distribution networks is fully looped,
197 this entails the entire network is included such as Modena; for other WDNs such as D-Town, only a
198 fraction of the network is selected (see supplementary information). The hierarchical organization
199 of smaller loops within larger loops can be quantified on two different levels: as a distribution of
200 measures for each individual node in a given tree, and also as an aggregate measure over the entire
201 tree.

202 **Nodal Measures** For the nodal level, there are two measures that have been previously developed:
203 the nesting ratio, and the partition asymmetry. For each node j in the tree, there are two branches,
204 r and s : branch r is the branch with a larger number of terminal nodes than branch s . The number
205 of terminal nodes contained in branch r is referred to as r_j , and the number of terminal nodes

206 contained in branch s is referred to as s_j . For each node j in the nesting tree, the nesting ratio is
 207 calculated as shown in Equation 2:

208
$$q_j = s_j / r_j \quad (2)$$

209 Where $r_j \geq s_j$ (so that q is a fraction less than 1) are the numbers of terminal nodes in branches r
 210 and s .

211 The partition asymmetry, also measured for each node in the graph, (referred to in the rest of
 212 the paper as asymmetry) has previously been introduced by [Modes et al. \(2016\)](#) and [Van Pelt et al.](#)
 213 ([1992](#)). It is calculated as shown in Equation 3 for a node j :

214
$$a(j) = \frac{r_j - s_j}{r_j + s_j - 1} \quad (3)$$

215 From Equations 2 and 3, it is clear that the nesting ratios and asymmetries calculated for a given
 216 tree would be inversely proportional, meaning high asymmetry values correspond to lower nesting
 217 ratios (i.e., less hierarchically nested loops).

218 **Network-Wide Measure** The aggregate tree-level measure has been developed and called the
 219 nesting number by [Ronellenfitsch et al. \(2015\)](#). The nesting number is an average of the nesting
 220 ratio distribution for a given tree and it decreases as the nestedness of loop hierarchy decreases.
 221 The nesting number is defined as a weighted average, shown in Equation 4:

222
$$i = \sum_j w_j q_j, \text{ where } \sum_j w_j = 1 \quad (4)$$

223 Both unweighted and degree weighted nesting number can be calculated: unweighted nesting
 224 number i_u , with $w_j = 1 \forall j$, and degree-weighted nesting number i_w , with weight, w , proportional
 225 to the subtree degree of a given node, j ($w_j \propto \delta_j - 1 = r_j + s_j - 1$, where δ_j is the subtree degree).
 226 A high value nesting number ($i_{u,w}$) qualitatively represents graphs that are highly nested.

227 In addition to the nesting number, from the obtained decomposition tree, this study evaluates the
 228 relationships among different measures such as loop subtree degree versus loop area, subtree degree

versus asymmetry, and subtree degree versus mean pipe radii to further characterize the loops of WDNs in the context of physical properties. The loop area is calculated as the physical-spatial area (in square meters), converted to a directly proportional measure of "square pixels". Mean pipe radii of a loop is the average pipe radius (in meters) of all of the pipes forming a given loop.

Quantification of Hierarchy: Pipe Diameter Gradation

Another measure of the network hierarchy quantifies the gradual change from larger diameter to smaller diameter pipes along flow paths, and Ronellenfitsch et al. (2015) and Modes et al. (2016) termed it Topological Length. Similar to asymmetry, the value is calculated for many segments of the network but can be evaluated as a network-wide measure by characterizing its distribution. Topological length is relevant to water distribution, because generally, abrupt fluctuations destabilize the system (Creaco et al., 2016). Due to the obtained type of distributions (power law), we define γ , as the power law exponent of a given topological length distribution for each water distribution network (Equation 5). The exponent γ allows capturing the power law distribution of topological length without bias as the mean would (see Faloutsos et al. (1999)).

$$P(L_e = l) \propto l^{-\gamma} \quad (5)$$

Where the frequency of a topological length, L_e , is a function of the topological length of the pipe raised to a power $-\gamma$. An exponent (γ) of larger magnitude indicates that pipes in a given water distribution network have a higher likelihood of having high topological length (see complementary empirical cumulative distribution plot in the supporting information) (Newman, 2005; Kunegis and Preusse, 2012). In other words, it is more likely to have paths with gradual change in pipe diameters, rather than abrupt change. The exponent γ is more accurate at capturing the behavior of the distribution than a mean or median because of the heavy tail (Faloutsos et al., 1999). The calculation procedure is described in detail in Modes et al. (2016) but in brief here: Starting from an initial pipe $e_1 \equiv < i_1, j_1 >$ between junctions i_1 and j_1 , we identify all the pipes e that are adjacent to it (share the node i_1 or j_1) and have diameter smaller than or equal to the diameter of pipe e_1 . We

choose the pipe with the maximum diameter from the set e , which is now e_2 , and add it to the trail, which now becomes (e_1, e_2) . The process is repeated for e_2 (identify all links that are adjacent to e_2 with diameter smaller than e_2 and choose the maximum) and iterate. The algorithm terminates when the set of pipes that have diameter smaller than that of the last link e_k in the trail is empty. The length of the trail associated with edge e_1 is $l(e_1) = k$. The process is iterative, starting from every pipe of the network, in this way associating a trail length $l(e)$ with every pipe e .

260 **Simulation-Based Performance Indicators**

261 *Hydraulic Simulation*

262 The selected performance indicators require hydraulic modeling of the networks. Different
263 kinds of hydraulic simulations can be conducted to calculate various WDN performance indicators.
264 In this study, pressure driven, extended period simulations were run for the range of demands for
265 24-hour duration (when demands are available). Pressure driven analysis was calculated using the
266 WNTR simulator within python (see [Klise et al. \(2017\)](#)). After conducting hydraulic simulations
267 using the WNTR package within python, both the entropy and the Todini index are calculated for
268 the water distribution networks using the WNTR package within python ([Klise et al., 2017](#)). Only
269 9 of the 15 networks are tested using the Todini index due to software limitations (i.e., a lack of
270 convergence in solving equations within reasonable time), but from the 9 available data points,
271 statistical validity is still established. For entropy, the data provided in [Santonastaso et al. \(2018\)](#) is
272 used to confirm obtained values.

273 *Entropy: Path Redundancy*

274 The entropy surrogate indicator assumes that greatest uniformity between supply paths to all
275 nodes minimizes expected shortfall in case of a pipe breakdown ([Tanyimboh and Templeman,
1993; Farmani et al., 2005](#)). Flows through pipes are obtained by simulating either a single demand
276 scenario or the average of an extended period simulation. This study uses the entropy gap, ΔS ,
277 meaning two simulations are conducted, one for the network with its current structure, and one
278 for the maximal path redundancy structure (i.e., structure with greatest supply path uniformity).
279 [Santonastaso et al. \(2018\)](#) proposed a measure of path redundancy, ΔS , which is akin to normalizing

281 the entropy of a given network by taking the entropy and dividing it by the maximum possible
 282 entropy given a network. By using ΔS , we can compare a given network's reliability to its ideal
 283 path redundancy. The equations for S , and ΔS are given in Equations 6 and 7 , as shown in
 284 [Santonastaso et al. \(2018\)](#):

$$285 \quad S = - \sum_{i=1}^{NS} \frac{Q_i}{T} \ln\left(\frac{Q_i}{T}\right) - \frac{1}{T} \sum_{j=1}^{NN} T_j \left[\frac{Q_j}{T_j} \ln\left(\frac{Q_j}{T_j}\right) + \sum_{ji \in N_j} \frac{q_{ji}}{T_j} \ln\left(\frac{q_{ji}}{T_j}\right) \right] \quad (6)$$

286 The first term is the entropy of supply nodes and the second is the entropy of demand nodes; NS is
 287 the number of supply nodes; T is the total supplied flow rate; NN is the number of demand nodes;
 288 Q_i represents the inflow at the i -th source node; T_j is the total flow rate reaching the j -th demand
 289 node; Q_j is the water demand at the j -th demand node; q_{ji} is the flow rate in the pipe connecting
 290 node j with surrounding node i ; and N_j is the number of pipes carrying water from the j -th demand
 291 node towards neighboring nodes. Similar to [Santonastaso et al. \(2018\)](#) , the maximization of S ,
 292 MS , is computed by the procedure proposed in [Yassin-Kassab et al. \(1999\)](#) and ΔS is calculated as
 293 follows in Equation 7.

$$294 \quad \Delta S = 1 - \frac{S}{MS} \quad (7)$$

295 *Todini Index: Power Surplus*

296 The Todini index, or resilience index, is found by simulating either a single demand scenario of
 297 a network or the average of extended period simulation. The simulation results provide the flows
 298 from reservoirs to nodes, the available head at each reservoir and demand node, and the power
 299 introduced by pumps in the system ([Dziedzic and Karney, 2014](#)). Again, though this measure
 300 provides surplus power available to be dissipated in the network in case of failure, it neglects how
 301 the system actually performs or recovers after a failure ([Farmani et al., 2005](#)). The Todini index
 302 evaluates excess pressure head available at junctions, and is calculated as shown in Equation 8
 303 ([Todini, 2000](#); [Dziedzic and Karney, 2015](#)):

$$304 \quad RI = \frac{\sum_{j=1}^n q_j (ha_j - hr_j)}{\left(\sum_{r=1}^R Q_r H_r + \sum_{b=1}^B P_b \right) - \sum_{j=1}^n q_j hr_j} \quad (8)$$

305 where n =number of demand nodes; q_j = demand at node j; ha_j = head available at node j; hr_j =
306 minimum head required to meet constraints at node j; R = number of reservoirs; Q_r = flow being
307 supplied to the system by reservoir r; H_r = head at reservoir r; P_b = power introduced in the
308 system by pump b; and B = number of pumps. The Todini index is intended to compare different
309 designs for the same network. As it does not always fall between [0,1], and the comparison with
310 hierarchical indicators is on a pipe-basis, the index is size-normalized by the number of pipes in
311 each network prior to conducting the regression analyses explained in the Results.

312 **Identifying Relationships Between Hierarchical Metrics and Performance Indicators**

313 After calculating both the entropy and the Todini index for the water distribution networks, linear
314 multi-regression analyses with both the nesting numbers (i) and topological length exponents (γ)
315 are conducted, using the *scipy* (Virtanen et al., 2020) and *seaborn* (Michael et al., 2018) packages
316 in python, to evaluate relationships between WDN hierarchy and hydraulic performance using R^2
317 and standard error (SE) .

318 **RESULTS AND DISCUSSION**

319 **Characterization of Hierarchy**

320 This study characterizes the distribution of subtree degrees of nesting tree nodes for each
321 network. Though subtree degrees are used as input for calculating loop nestedness measures, it
322 is beneficial to understand the type of distribution subtree degrees follow to gain insight on the
323 organization of loops. For the most part, subtree degree distributions for all water distribution
324 networks are significantly approximated by a power-law distribution, $p \ll 0.05$. Only very small
325 networks, such as TLN are not considered, because they do not have enough data to estimate a
326 distribution at all (e.g., only 2 points). The distribution for Net6 is shown in Figure 2. The linear
327 relationship on the log-log scale of Figure 2b indicates power-law behavior. See supplementary
328 information for the remaining graphs. We also characterize the distribution of topological lengths
329 for each network. For the most part, they are all significantly approximated by a power-law
330 distribution. After confirming their significant power-law distributions, with ($p \ll 0.05$), using

331 methods described in [Clauset et al. \(2007\)](#), we store the power law exponent, γ , characterizing each
332 network's distribution. Again, only very small networks, such as TLN are not considered, because
333 they do not have enough data (only two data points). The distribution for Net6 is shown in Figure 3.
334 The linear relationship on the log-log scale of Figure 3b indicates power-law behavior. Individual
335 figures for a given network are shown in supplementary information. These findings are interesting
336 because node-based topological measures accounting for nodal degree and other centralities of
337 water distribution networks often follow poisson distribution rather than a power-law (([Giustolisi
338 et al., 2017](#)) among others). If water distribution network component connectivity follows a poisson
339 distribution, that implies the networks are generally robust to targeted and random modes of failure
340 (i.e., criticality and vulnerability is relatively randomly distributed among components). Whereas
341 a power-law distribution indicates that there are few components that are especially critical or
342 vulnerable, such that their failure may be catastrophic for the given network. This study suggests,
343 from the approximate power-law distributions, that perhaps water distribution networks do not
344 always follow a poisson distribution with respect to some key properties (e.g., loops), and thus
345 are not necessarily immune from targeted modes of failure. These findings are consistent with the
346 observation of power-law type of hierarchical behavior that is observed in other urban infrastructure
347 networks ([Yang et al., 2017](#); [Krueger et al., 2017](#); [Klinkhamer et al., 2019](#)) and previous research
348 on water distribution networks ([Abdel-Mottaleb and Zhang, 2019](#)).

349 **Physical Context**

350 *Subtree Degree versus Loop Area and Asymmetry*

351 This study also examined relationships between subtree degree of loops and the corresponding
352 loop area and asymmetry. As shown in Figure 4(a, c, e, g, and i), higher subtree degree nodes
353 correspond to loops with larger areas (i.e., smaller loops have smaller subtree degree). At the same
354 time, there are generally more data points (i.e., nodes or subtrees) concentrated in the smaller loop
355 area and smaller subtree degree space of the plots shown in Figure 4. This indicates that water
356 distribution networks generally have more smaller loops than larger loops. As shown in Figure 4(b,
357 d, f, h, and j), for many networks, the higher the subtree degree, the higher the asymmetry of a

358 given node. However, this observation is not consistent for all of the water distribution networks.
359 For many of the tested networks, there is a decrease in asymmetry near the mid-range of subtree
360 degree. Given that the subtree degree of a loop is closely related to its physical area, it seems
361 that loops of mid-range area are more hierarchically nested than larger area loops. The reason
362 for this may be that larger loop redundancies are more expensive and less feasible than adding
363 redundancies (and thus more nestedness) to smaller loops. This suggests a tradeoff between adding
364 less expensive redundancies (at the smaller loop level) and adding redundancies that will serve
365 more of the population (i.e., larger distribution mains). There also seems to be a larger spread of
366 asymmetry values for smaller subtree degrees and thus smaller area loops may contain either highly
367 evenly or unevenly distributed redundancies. However, path redundancies are not solely quantified
368 using the asymmetry, nesting ratio and nesting numbers. There are other factors interplaying with
369 these measures of nestedness, such as source location and pipe diameters.

370 *Source Location and Subtree Degree versus Mean Pipe Radii of a Loop*

371 Though previous research has quantified shape (e.g., grid, branch, loop) of water distribution
372 networks, such as [Hernandez et al. \(2016\)](#), there remains a gap of accounting for water sources
373 in research on water distribution network structure ([Giustolisi et al., 2017](#); [Meng et al., 2018](#);
374 [Giustolisi et al., 2019](#)). Location of the water source influences whether larger pipes are on the
375 outer, larger loops, or whether larger pipes are within smaller internally nested loops. Hence this
376 study further examined the relationship between degree and mean pipe radii; differences in the
377 relationship between these two properties of the decomposition tree may be attributable to demand
378 allocation and source(s) placement. Not all studied water distribution networks have the same
379 relationship between subtree degree (and consequently, loop area) and mean pipe radii of that
380 subtree (i.e., loop). In Figure 5, five plots of subtree degree versus mean pipe radii are shown (see
381 supplementary information for remaining plots).

382 From Figure 5e and f, Fossolo's larger diameter pipes are not part of the largest loop, whereas
383 they are for Net3 (5c and d) and Modena (5a and b). Because Fossolo has a single water source,
384 pipe diameters are not as uniform throughout the network as they are for multiple source networks

(e.g., Net3 and Modena). Another observation is that larger pipes are on the periphery of the Modena, Net3 and D-Town networks, whereas for Net6, the largest diameter pipe is not even in the largest looped part selected for analysis. Similarly, the degree versus asymmetry distributions for Modena and Net3 are much closer in distribution shape than they are to Fossolo and Net6 (even low degree loops in Fossolo and Net6 show high asymmetry, whereas only the highest degree loops show highest asymmetry in Net3 and Modena). This observation is confirmed upon calculating the Kolmogorov-Smirnov statistic between the asymmetry distributions of the networks, following the method in [Ronellenfitsch et al. \(2015\)](#) (see supplementary information). It is interesting that for these five networks, the nesting number, shown in Table 1, is higher for networks with the highest mean pipe radii on the periphery of the largest looped part. In addition, both Net3 and Modena have multiple sources, whereas Fossolo has a single water source that no doubt influences pipe size along the gradient of larger area to smaller area loops within the network (i.e., the location of the source(s) of water, and number of sources influences the distribution of pipe diameters relative to the networks' loops). Multiple storage tanks in a network, depending on their placements relative to the demands, can result in increased entropy or pathway redundancy, as the pipe diameters can be smaller than they otherwise would have to be if there weren't as many source redundancies ([Chin et al., 2000](#); [Walski, 2000](#)). These observations open the question of how physical network components (e.g., number and location of sources) influence the hierarchy, and consequently performance, to manage network maintenance and operations.

Relationships Between Hierarchy and Performance

There is a significant correlation between the network hierarchy and simulation-based performance indicators. For entropy, in the normalized form (ΔS), smaller values (i.e., closer to zero) indicate a network is closer to its “ideal” or maximal path redundancy. First, a regression analysis is conducted between the baseline topological measure of meshedness, r , and ΔS . The significant R^2 value of 0.3 indicates that there must be other factors influencing the path redundancy in addition to the ratio of existing to maximal potential number of loops. Meshedness alone is limited at capturing path redundancy in water distribution networks. Though meshedness has been shown

412 to be a robust measure of path redundancy (Yazdani and Jeffrey, 2011), it is limited in explaining
413 variability observed in the gap between actual and optimal path redundancy ($R^2 = 0.3$). However,
414 when a multi-regression is run with the nesting number, the R^2 increases to 0.63. The R^2 further
415 increases to 0.83 when the pipe diameter gradation is included. When the pipe diameter gradation
416 is included, the number of samples decreases to 14 because two of the networks do not have enough
417 data points to calculate γ (still, the results are significant with greater than 95 percent confidence,
418 $p \leq 0.0003$). Regardless, this indicates that, not only the pipe-junction topology of a WDN impact
419 its flow path redundancy, but so does its loop and pipe diameter hierarchy.

420 Networks with higher nesting number values (i.e., more nestedness and loop symmetry) tend
421 to have a significantly lower gap between their actual and maximum entropy values, ΔS (Figure
422 6a). The pipe diameter gradation measure (γ) also has the same effect on ΔS , but stronger (Figure
423 6b). However, when evaluating their impact on the Todini index (excess pressure head at junctions,
424 or energy redundancy), the nesting number and pipe gradation displayed different relationships.
425 The nesting number of a network did not have as significant of a relationship with the Todini
426 index (Figure 6c), but higher values of γ , pipe diameter gradation, increased the Todini index
427 (Figure 6d). Higher values of the exponent, γ , indicate more gradual changes in diameter in
428 the network. Pipe diameter gradation along flow paths, γ , explained the variability in the Todini
429 index ($R^2=0.856$, $n=9$, $p \leq 0.001$, $SE = 0.010$) more than that observed for entropy ($R^2= 0.66$,
430 $n=15$, $p \leq 0.005$, $SE = 0.053$). However, when meshedness, loop nestedness and pipe diameter
431 gradation are accounted for, the correlation significantly increases ($R^2=0.83$, $n=15$, with $p \leq 0.001$,
432 $SE = 0.039$). This supports the hypothesis that hierarchy of loops and pipe diameters influences
433 the two tested performance indicators (i.e., is an integral part of WDN structure). However, actual
434 performance for WDNs depends not only on their pipe-junction or hierarchical representations, but
435 also on operational, design, and dynamic conditions that are not considered in this work (but can
436 be included in future studies).

437 Increasing loop nestedness has leverage on path redundancy, whereas more gradual pipe dia-
438 meter change can simultaneously enhance path redundancy and power surplus (or energy redundancy).

439 This suggests that WDN design optimization can be improved by including decision variables re-
440 lated to pipe diameter gradation along flow paths. Previous studies have focused on optimizing the
441 design of WDN loops or sizing pipes without considering diameter gradation along paths (([Todini, 2000](#);
442 [Creaco et al., 2016](#); [Dziedzic and Karney, 2015](#)) among others). Though [Creaco et al. \(2016\)](#)
443 took it further by considering diameter gradation of loops, it does not extend to flow paths. When
444 diameter gradation is accounted for even just within loops, [Creaco et al. \(2016\)](#) found additional
445 solutions to WDN design optimization problems. Instead of solely focusing on adding loops or
446 maintaining diameter uniformity of loops to enhance WDN redundancy and subsequent reliability,
447 effort should be made to increase the pipe diameter gradation along paths throughout a network for
448 increased leverage.

449 CONCLUSION

450 We characterize WDN hierarchy, showing that loop nestedness (i.e., subtree degree) and pipe
451 diameter gradation along flow paths (i.e., topological length), are approximated by power-law
452 distributions. This indicates that WDNs are more vulnerable at the loop level than at the junction
453 level. With respect to network design, differences in the relationships between location of larger
454 pipes and nestedness, and loop area and nestedness were observed based on water source location,
455 suggesting that hierarchical indicators capture more information regarding water source location
456 than pipe-junction topology. This study also found that the hierarchy of WDNs, as quantified by loop
457 nestedness and pipe diameter gradation along flow paths, explained variability of simulation-based
458 performance indicators (specifically flow path redundancy and power surplus). Quantifying and
459 characterizing the different representations of WDN structure is a necessary step before applying
460 structural measures in network optimization, failure analysis, and design/scenario comparisons.

461 There are however several limitations to the study that can be addressed in future work. The
462 nesting number, or measure of loop nestedness, used in this work captures the largest looped
463 part, and not the entirety of the network. This limitation can be addressed in future work by
464 modifying the measure to account for more loopy parts. This study analyzes the network as a
465 single snapshot (i.e., static not dynamic as it actually is). The hierarchy of components may

466 likely change as water distribution infrastructure co-evolves with cities. Real WDNs must also
467 be analyzed to confirm the identified relationships before hierarchical indicators are adopted to
468 estimate surrogate performance indicators. Nonetheless, analyzing the hierarchical representation
469 of WDNs adds much more insight on their structure that contributes to the hydraulic performance
470 than only analyzing their pipe-junction topology.

471 **DATA AVAILABILITY STATEMENT**

472 • All data, models, or code generated or used during the study are available from the corre-
473 sponding author by request.

474 **ACKNOWLEDGEMENTS**

475 This material is based upon work supported by the National Science Foundation under Grant
476 Number 1638301. Any opinions, findings, and conclusions or recommendations expressed in this
477 material are those of the authors and do not necessarily reflect the views of the National Science
478 Foundation. N. Abdel-Mottaleb thanks Dr. Henrik Ronellenfitsch for his generous help in using
479 the Nesting python package. All water distribution networks are publicly available, with sources
480 cited in paper. All software used to obtain data and analyze results is open source and also cited in
481 the paper.

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657 Pittsburgh, Pennsylvania, 484–497.

658 **List of Tables**

659	1	Measurements of r (meshedness), size-normalized RI (Todini Index, energy redundancy), ΔS (entropy or path redundancy gap), γ (topological length distribution exponent), and i (nesting number) for WDNs	29
660			
661			

TABLE 1. Measurements of r (meshedness), size-normalized RI (Todini Index, energy redundancy), ΔS (entropy or path redundancy gap), γ (topological length distribution exponent), and i (nesting number) for WDNs

Network	r	RI (size normalized)	ΔS	γ	i
Anytown	0.422	–	0.121	0.621	0.365
Net1	0.176	0.0900	0.106	1.128	0.813
Net2	0.075	0.0125	0.127	0.618	0.700
Net3	0.121	0.0053	0.144	0.634	0.486
Net6	0.080	0.0001	0.203	0.537	0.164
Fossolo	0.318	0.0236	0.128	0.772	0.386
Modena	0.085	0.0008	0.162	0.570	0.531
Pescara	0.201	–	0.139	0.617	0.534
Richmond	0.049	–	0.181	0.428	0.649
D-Town	0.065	–	0.169	0.632	0.762
TRN/Gessler	0.315	–	0.108	0.825	0.435
ZJ	0.228	0.0000	0.147	0.573	0.791
Rural	0.126	0.0018	0.167	0.428	0.688
Jilin	0.137	0.0000	0.122	0.613	0.829
TLN	0.222	–	0.098	–	0.700