Condensing Complexity

K-means clustering of geometric data sets as a design tool

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This paper explores the use of K-means clustering as a design tool to manage geometric complexity in design contexts. While computational design has often been associated with formal complexity, this work investigates techniques for condensing complexity and structuring irregular datasets into meaningful clusters to enable systematic design interventions. By applying K-means clustering to irregular geometries, the paper demonstrates how digital abstraction can serve as an alternative to physical standardization, preserving material and/or geometric specificity in structured assemblies. Three case studies illustrate different approaches to integrating clustering within design systems, highlighting its potential to enable informed design decisions.

Keywords: *K-Means Clustering, Discrete Design, Stock-Based Design, Geometry Rationalization.*

INTRODUCTION

From their early adoption ca. 30 years ago, computational design tools have been associated with the development of design systems and artifacts of high complexity, with the aim of developing responsive geometric systems able to adapt to different external factors, as well as a specific interest for complex formal aesthetics (Schumacher, 2011). As a response to such interest in formal complexity, researchers proposed the concept of "simplexity" (Michalatos and Kaijima, 2008), based on the idea of building a practical system by breaking down complexity and hence allowing designers form a more intuitive understanding of it. This paper follows in this research by proposing computational techniques to "condense" the inherent complexity associated both with material-specific geometries and digital data, developing tools to enable designers to reduce and increase complexity of the digital representations they work with according to their needs.

BACKGROUND

When looking at design logics working with different degrees of geometric complexity, this paper reviews the tension existing between discrete combinatorial logics and material variation, and surveys existing computational strategies for the management of such tension.

Between discrete and material-specific logics

In recent years research grouped around the concept of the "discrete" proposed design methods based on the aggregation of modular parts, aiming at providing a more open and accessible design and fabrication system (Retsin, 2019; Rossi, 2023). The discrete advocates for decentralized and democratic production, but as with most digital design methods

it still relies on the fabrication (of parts) from new materials. However, in the context of reused material stock such systems are difficult to implement, especially when dealing with non-standard materials, as discrete systems strongly rely on standardization of the parts. Similarly, when working with complex design information as input, such as in the case of performance-driven design processes, discrete design methodologies often fail to provide sufficient adaptability to reconstruct the design input with sufficient fidelity.

To respond to this and to provide more material-informed design strategies, in recent years researchers proposed different techniques for stock-based design (Cousin et al. 2023, Allner, Kröhnert and Rossi, 2019). The material stock is assumed as the starting point rather than as the final outcome, hence allowing to account for the unique geometric and material characteristics of found artifacts. Many of the studies in this context rely on reducing complexity of the input elements through physical editing of elements to adapt to a digital design model (Devenes et al., 2022), partially wasting material and losing some of the design potential embedded in the artifacts.

Computational techniques for management of geometric complexity

In existing computational design research, there are examples of different approaches to managing the geometric complexity of unique artifacts. Several relevant examples in this context work with the unique geometries of wood branches, aiming at avoiding or reducing waste when working with non-linear timber elements (Mollica and Self, 2016). In this context, different projects explored degrees of geometric representational complexity, ranging from models including only centerlines (Allner, Kröhnert and Rossi, 2019) to others using the full geometry of the wood elements (Moreno Gata et al. 2024).

When it comes to matching such complex geometries to an existing design goal, techniques have been proposed which often rely on the use of assignment algorithms, such as the Hungarian method (Kuhn, 1955). Such algorithm has been used for different applications, ranging from the reuse of concrete elements (Eschenbach et al. 2022) to the above-mentioned wood branches problem (Amtsberg et al. 2020), and other material-specific reuse strategies (Cousin et al. 2023). However, it must be noted that the Hungarian method relies on relatively complex computational implementation, which makes it not always suitable in a design context.

For this reason, the use of K-mean clustering algorithms to reduce the complexity of the input stocks has been proposed to enable the use of simpler combinatorial design tools for the generation of assemblies (Allner, Kröhnert and Rossi, 2019). K-means clustering is a common technique used to group elements according to their similarity and has been used in architecture for applications such as panels variation reduction in facade design (Pena de Leon, 2012). While implementations of the algorithm exist for use in computational design (Zwierzycki, 2023; Miller, 2024), the need for customization and easy access to the algorithm required a custom implementation.

CONTRIBUTION

Discrete element aggregation methods aim for versatility in the combination of parts rather than the variability of parts themselves (Retsin, 2019) and therefore perform best with a small variation of data input. Against this background, and to bridge the gap between real-world complexity and the simplicity required by such systems, K-means clustering is proposed as a design methodology for reducing the geometric complexity through digital abstraction. This approach is explored through three case studies: two that use stock elements as building parts, and one that focuses on the discretization of FEA-derived stress lines to build an optimized slab panel from simple elements. All projects use the discrete element aggregation method to assemble non-hierarchical structures of modular parts, demonstrating how the design input can be

simplified, while preserving the specificity of unique input geometries.

METHODOLOGY: CLUSTERING AS AN ABSTRACTION/DESIGN TOOL

This section outlines the main characteristics and the custom implementation of the K-Means clustering algorithm proposed in this work.

K-means++ clustering: concept and parameters

K-means clustering is a widely used iterative unsupervised learning algorithm that partitions a dataset into clusters of similarity (similar data points). The algorithm has two main objectives: minimizing variance within each cluster (ensuring items within a cluster are as similar as possible) and maximizing variance between clusters (ensuring clusters remain distinct from one another). A practical example of a clustered set of bicycle frames can be seen in Figure 1.

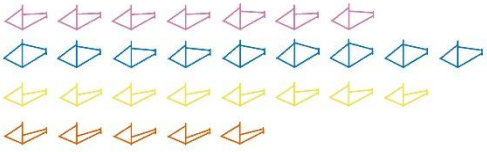

Figure 1
Exemplary set of clustered bicycle frames

The three most important parameters influencing the clustering outcome are the initial selection of cluster centroids, the number of clusters (k value), and the dataset (feature vector) itself.

Initial selection of cluster centroids. In the standard algorithm (naïve K-means), cluster centers are randomly chosen from the dataset and iteratively adjusted until the algorithm converges. Due to the random selection sometimes inadequate results are produced. A significant improvement to this problem is K-means++, proposed by Arthur and Vassilvitskii (2007), which ensures that initial cluster centers are more evenly distributed across the dataset, reducing probability of poor clustering outcomes.

Number of clusters (k value). A higher k value results in smaller clusters with lower intra-cluster variance, while a lower k value produces larger clusters with higher intra-cluster variance. Selecting the optimal number of clusters is not a straightforward task, as there is no single best solution. In a design context, manually and intuitively determining k based on design intent is often the most productive approach. However, various methods can assist in selecting a reasonable k-value. One prevalent strategy is the elbow method, an approach to identifying an “optimal” number of clusters by detecting a kink (elbow) in the value distribution graph. While the elbow method can be useful, it is not ideal, especially for datasets with high dimensionality or irregular shapes (Schubert, 2023).

A more effective visual aid for determining a suitable number of clusters is the use of curve or box-and-whiskers plots to analyze the variance distributions within each cluster (Figure 2). In this example axis models of 3D scanned tree branches are analyzed. When clustering objects that share the same topology but exhibit geometric irregularities, an average geometry can be computed, allowing to measure the deviation from this "proto-part."

The graphs in Figure 2 illustrate geometric deviation of 238 elements relative to their averaged geometry as a box-and-whisker plot. Comparing the results for two (upper) and six clusters (lower) to the non-clustered dataset (black), the results indicate that with only two clusters, the deviation ranges (8–182mm, 0–145mm) remain nearly as broad as in the non-clustered set (0–225mm). In contrast, six clusters significantly reduce deviation, five stay below 100mm, and only one is slightly higher, mostly aligning with or staying below the average deviation of the non-clustered set.

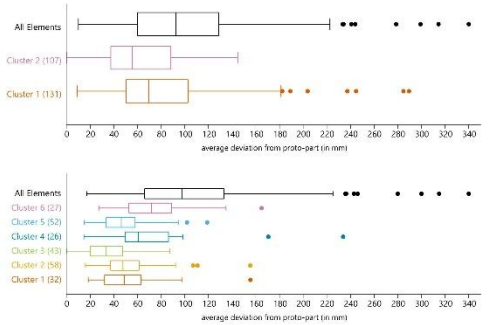

Figure 2
Box-and-whisker plots showing the remaining intra-cluster variance for different k values in a set of 238 branch axis models

Dataset structure (feature vector). One of the advantages of using K-means clustering is its ability to handle multiple objectives simultaneously. In the context of clustering geometric objects, multiple properties—such as size, weight, material, etc.—can be considered in combination when determining similarity, rather than relying on a single aspect (e.g. size alone). This set of properties is commonly referred to as a feature vector.

Feature engineering for clustering in design

To illustrate the potential of feature engineering in clustering geometric objects, the dataset of 238 3D-scanned Y-shaped tree forks as simplified axis models is used. The dataset exhibits significant variation, with overall fork lengths ranging from 22 cm to 195 cm. The cross-sections of the three branch segments vary between 3.5 cm and 16.3 cm in diameter. Three different feature vectors and their respective clustering results are compared to evaluate the clustering "success" in relation to the selected geometric features.

In the clustering process, a tree fork can be mathematically represented through various geometric attributes, such as overall shape (approximated by centerlines), size (branch segment lengths), angles between the three branching segments, and cross-sectional radii. To ensure comparability between different clustering results, modifications to the standard K-means++ algorithm were necessary. Specifically, both the initial cluster center and the random seed used for placing additional cluster centroids were fixed to predefined values instead of being randomly assigned. The number of clusters was kept constant, and all data was normalized for the algorithm to work efficiently.

Figure 3 illustrates a subset of the complete set of tree forks. These are clustered using three different feature vectors:

- Left: based solely on the three angles that define the Y directions of each fork. These are measured from the central node to a point on each centerline, either 50 cm away from the node or, if shorter, at the endpoint.
- Middle: the three angles and the three cross-sectional radii of the branch segments.
- Right: the three angles and the overall shape of each fork, with shape represented by 20 evenly spaced points along each branch arm's centerline.

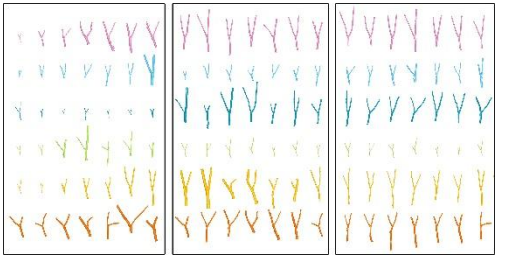

Figure 3
Clustering results (focusing on a subset of elements for visualizing purposes) of different feature vectors. Items in each colored row belong to one cluster

When clustering is based only on angles (left), it is immediately apparent that each cluster still contains forks with considerable variation in size and cross-section, comparable to the range of the non-clustered set. Introducing additional geometric features significantly reduces variance within each cluster. In the middle example, where both angles and cross-sections are considered, the most noticeable outcome visually is the remaining variance in overall size within each cluster. When clustering is based on angles and shape (right), the

results show a clear separation of larger and smaller branches into different clusters.

A closer examination reveals that clusters also differentiate between shape similarity, separating narrower and wider shapes, as well as different (length) proportions. The effectiveness of the process can also be evaluated quantitatively, as described previously. Focusing on the clustering results achieved with a feature vector combining angles and cross-sections (Figure 3, middle), the

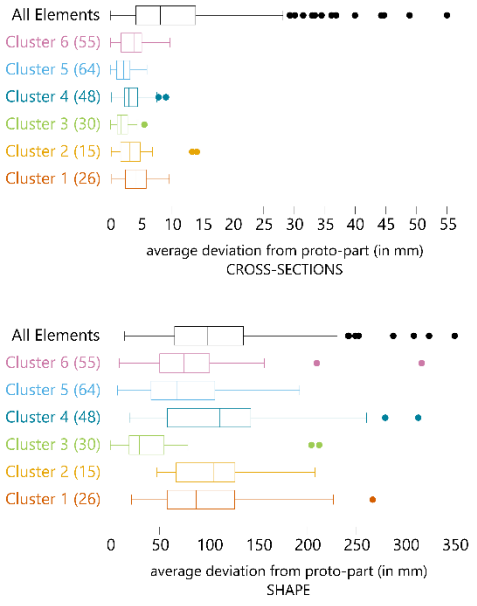

Figure 4
Box-and-whisker plots displaying the remaining intra-cluster variance regarding cross-sections (top) and overall shape (bottom), feature vector combining cross-sections and angles

Figure 5
Geometric average (proto-part) of five exemplary clusters of tree forks

degree of variance within clusters can be analyzed mathematically. The charts in Figure 4 illustrate that the variance in average radius of the cross-sections (top) within each cluster is significantly reduced (0-10mm) compared to the non-clustered dataset (0-28mm), excluding outliers. In contrast, the variance and range of shape deviation (bottom) remain large and comparable to those of the non-clustered set.

Defining cluster representations

Clusters from an inventory of diverse parts can be represented by a "proto-part", which is the average geometry of elements in each cluster. This approach significantly reduces the complexity a designer must navigate, while preserving key geometric features.

In both case study examples that address the reuse of found objects, the representative averaged proto-parts are calculated based on centerline models. Figure 5 illustrates five exemplary proto-parts (bold lines) derived from their respective clusters (thin lines) for tree forks.

CASE STUDIES: CLUSTERING IN DIFFERENT DESIGN CONTEXTS

This section outlines three case studies, each demonstrating applications of the described geometry reduction method in a design context.

Case study 1: tree forks

Using the example of a table frame design, Y-shaped tree forks are connected in alignment with their fiber directions. This approach builds upon existing exploration of naturally grown wood elements as structural components (Mollica and Self, 2016, Allner, Kröhnert and Rossi, 2019). For this design task, six such elements are required to form the smallest stable frame, as illustrated in Figure 6, creating three legs and three connection points supporting the tabletop.

A conventional approach might be to select and arrange the forks in a way that produces as many similar tables as possible. One strategy for achieving this would be to cluster the forks by shape and angles into six groups. However, due to the large geometric range of organic elements, K-means clustering typically returns clusters containing an uneven number of elements. If each table is to be constructed using one fork from each cluster, the

maximum number of tables that can be built is only 26, leaving 82 elements (~ one-third of the inventory) unused.

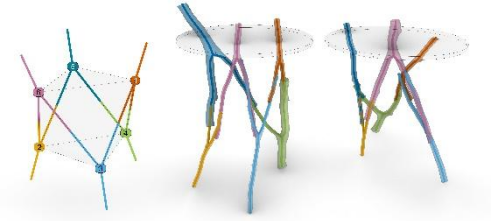

Figure 6
Topology for a table design from six Y-shaped tree forks (left) and two exemplary tables from elements from the inventory

Another important factor is the weights distribution within the feature vector itself. In this case, it contains 180 data points related to shape (60 points × 3 coordinates), but only three values each for angles and cross-sections. As a result, shape dominates the clustering process, leading to groups of rather small and thin forks, and ones containing larger and thicker ones. When assembled into a table, these variations result in mismatched diameters and uneven transitions between elements (Figure 6).

A more effective way to interpret the clustering results as design input is to prioritize intra-cluster design rather than forcing a cross-cluster combination that does not reflect the actual properties of the elements. In the second test, the feature vector was adjusted to emphasize spatial and structural properties more effectively. It combined the three angle values, the two most relevant cross-section diameters for this design intent, and a single value representing the average segment length of each fork's three arms. This weighting ensures that angles remain the highest priority, while size has the lowest influence—recognizing that larger tree forks can easily be trimmed to the required dimensions during fabrication. By prioritizing spatial orientation and cross-sectional continuity, the clusters naturally guide a design that respects the inherent characteristics of the material.

The outcome is no longer a set of identical tables but rather a diverse range of tables and stools that share the same topology but vary in size and proportion to accommodate different uses and users (Figure 7).

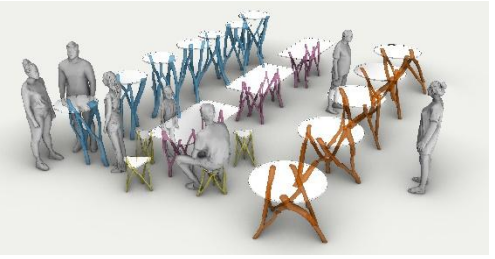

Figure 7
Possible variations of the same table frame topology build from tree forks belonging to the same cluster (per color)

Case study 2: reuse of bicycle frames

In a second study in the context of reuse, a set of bicycle frames is tested. As in the previous example, parts from an inventory are assembled according to a predefined pattern to form a larger lattice structure. Existing joints in the bicycle frames, originally intended for saddle or wheel connections, are used for connection to leverage the embedded technical potential of the artifacts (Figure 8).

Figure 8
Two bicycle frames joined by a steel rod using the existing standard connections

These predefined joints, each with a specific axis direction, serve as the main criterion for aggregation. Patterns are initially designed using identical proto-parts, which are later replaced with unique inventory parts. Due to geometric variation, joint axes become misaligned. Physics simulation in Kangaroo 3D (Senatore and Piker, 2015), reduces these misalignments, though some deviation remains.

Attempts to find more optimal constellations using brute-force yielded only marginal improvement with high computational cost. Alternatively, K-means clustering was tested to order the parts layout within patterns.

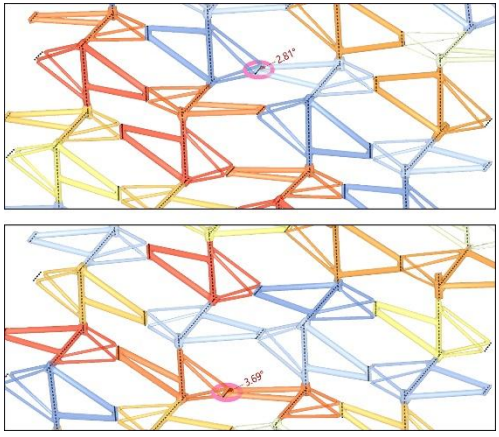

Figure 9
Best performing combination of proto-parts in pattern C (top), and best performing constellation of randomly placed proto-parts (bottom)

Analysis of two example pattern designs showed that the greatest deviations occur where geometrically diverse frames are positioned closely. Both patterns follow a periodic structure, combining linear sequences into lattices. Local geometric differences within these sequences disrupt continuity and cause misalignments. To address this, proto-parts from a clustered set are first distributed along these sequences. This orderly distribution of parts in rows across patterns enforces the periodic pattern structure and reduces joint angle deviations compared to random part distributions.

In pattern A, a distribution of proto-parts in "vertical" rows tested in 50 configurations resulted in an average maximum deviation of 0.37°, compared to 1.45° for random layouts. In pattern C, diagonally arranged proto-parts showed average values of 4.4° compared to 5.5° in random distributions (Figure 9). Although improvements are minor, they could still be significant considering the tight tolerances in steel construction.

Case study 3: discretization of FEA-derived stress lines

The last case study demonstrates the effectiveness of K-means clustering in facilitating the interpretation of complex geometric data generated through Finite Element Analysis (FEA). Principal stress lines, derived from structural simulations, serve as indicators for the development of material efficient structures by referring to force flow and identifying zones of high stresses. Accurately capturing these trajectories typically requires high-resolution meshing, which in turn produces large volumes of line data. While regions with dense line distributions can often be identified intuitively and approximated manually, such approaches are inherently imprecise and become impractical when processing multiple FEA datasets.

To address this challenge, K-means clustering was employed as a computational strategy to reduce geometric complexity and to identify salient patterns within the distribution of stress lines (Figure 10).

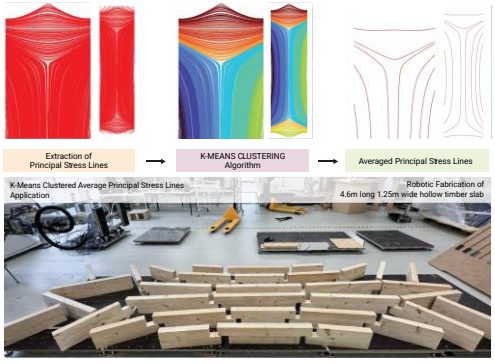

Figure 10
Averaged curves of K-Means clustered principal stress lines from FEA, applied to a robotically fabricated hollow timber slab system

The data structure was designed to be extensible, supporting the inclusion of various parameters such as the coordinates of division points along curves, curvature values, and deviation metrics. In two-dimensional analyses, only 2D coordinates were utilized; however, the framework is readily extendable to three-dimensional clustering tasks. This adaptable methodology enables efficient

abstraction and pattern recognition across varying spatial dimensions and scales of geometric data, thereby contributing to the automation and scalability of structurally informed design workflows.

RESULTS & DISCUSSION

This section discussed the impact of the developed clustering process for combinatorial design logics, and the role of the designer.

Clustering as a tool for complexity reduction

The case studies illustrate different approaches to "condensing" complex information to facilitate discrete design systems in both bottom-up (case 1 and 2) and top-down workflows (case 3). This simplification provides an interface for designers to utilize this information in design workflows.

To work on aggregations of discrete elements with tools like Wasp (Rossi and Tessmann 2019), reducing complexity is essential for limiting the design search space. A system based on a single proto-part often fails to accommodate diverse inventories, leading to mismatches when proto-parts are replaced by actual specimens. Conversely, using only unique irregular elements creates impractical design systems. Clustering elements into groups, each represented by a proto-part, offers a balanced approach, reducing variation, simplifying rule definition and improving part matching, making reuse of irregular elements more manageable.

While industrial artifacts like bicycle frames show limited variation, clustering still helps manage differences. However, its full potential lies in applications with datasets with greater diversity. Rather than just optimizing predefined patterns, clustering could be used earlier in the process to generate new pattern designs from different part types identified via clustering. In such a process, clustering could become an integral part of reuse design, rather than being only used for post-design optimization. In more top-down design approaches, as in the case of the stress-lines discretization, the reduction of complexity through clustering is also effective, allowing the use of vector fields to guide placement of discrete parts.

These approaches show the potential of k-means clustering as a design tool. Its ability to detect types within data sets makes it an ideal complement of discrete design bridging the gap between gradual differentiation (in the physical world) and modularity.

The role of the designer: algorithmic control and geometric agency

The comparisons between using different feature vectors on the same dataset in case study 1 demonstrate how feature selection directly shapes clustering outcomes. By determining which aspects of an object to prioritize, designers can tailor the clustering process to align with structural, aesthetic, or material considerations. This approach enables the development of an inventory-based design system that integrates both bottom-up methods, where the inherent features of the elements inform the design, and top-down strategies, where the designer defines which features influence design outcomes and how elements are connected topologically.

In case study 3, feature vector design defines the resolution of the design space to match the simplification of a force field to the scale of modular units to adequately inform an assembly. The ability to cluster based on multiple criteria proves valuable when selecting stock elements for architectural reuse. It allows for an accessible and productive material-driven design strategy mediating between designer's intent and physical reality and potential of the available material stocks. This shifts the design process away from a traditional top-down approach – where form is imposed into material – towards one centered on curating information and feature engineering within a given set. The stock parts are granted a degree of agency, influencing the design outcome rather than merely serving it.

CONCLUSION & OUTLOOK

Using clustering for conditioning discrete design systems can help to expand the applicability of such design methodologies. Non-standard artifacts can be implemented as modular parts, making it a useful tool for reuse and the circular economy, and modular discrete assemblies can be adapted to real world conditions via abstracted data maps, making it possible to achieve complex optimization with simple means.

K-means clustering remains one of the most widely used clustering algorithms, due to its accessibility and ease of implementation. It is computationally efficient and always produces a result, which can give the impression of a definitive solution, even as no truly optimal clustering exists. As Schubert (2023) points out, K-means is an exploratory method rather than an optimization tool, yielding multiple possible solutions whose usefulness is ultimately a user-driven decision. This makes it suited for creative applications in the context of design and architecture based on stock elements (Figure 11), where it can help to generate new approaches, rather than strictly optimizing geometry.

However, determining an adequate number of clusters remains a critical challenge. More robust and adaptable methods should be explored. Additionally, alternative clustering algorithms potential, such as spectral clustering, Gaussian mixture models, and DBSCAN could be evaluated for design applications. Further areas of research include the integration of automated methods for determining the number of clusters. Such advancements could enhance the use of clustering in discrete design workflows, bridging between algorithmic control and intuitive decision-making.

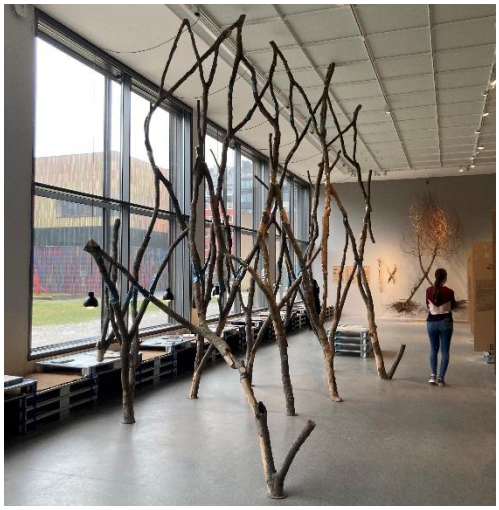

Figure 11
Spatial structure from 75 unique beech branch forks. Part of the "Trees, Time, Architecture" exhibition at the Architekturmuseum der TUM, Munich, 2025

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