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Mechanics-Guided Member Grouping for Cross-Section Optimization with Heterogeneous Graphs

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Abstract

Structural member sizing directly influences material consumption, embodied carbon, and overall structural efficiency. Recent advances in graph representations have opened new possibilities for structural optimization, with applications such as topology optimization and surrogate modeling. We propose a graph-based representation learning and clustering pipeline that uses structural simulation results to support member sizing and cross-section optimization. In this representation, connection points and linear members in the structural system are modeled as two node types in a heterogeneous graph. Mechanical responses, geometric properties, and topological information are encoded as features, and structural context is propagated through message passing. We then train a Heterogeneous Graph Attention Network (HeteroGAT) encoder with a contrastive objective constructed from mechanically similar and topologically adjacent member pairs. Finally, we cluster the learned embeddings with Gaussian Mixture Models (GMM). The resulting clusters provide a practical basis for structural optimization. Specifically, we use the clustering results as grouping rules for cross-section optimization in Karamba3D, such that members within the same cluster share a common profile. Using steel member sizing as a case study, we evaluate the cross-section assignment strategies on a whole-building structural system and demonstrate the method through multiple application examples. The results show that the proposed method achieves a rationalized section system with significantly fewer cross-section types and stable convergence, while maintaining structural performance comparable to the original design, making it a practical tool for early-stage steel structural design.

Keywords: graph neural network (GNN), structural optimization, heterogeneous graphs, mechanics-guided clustering

1. Introduction

The construction industry is one of the largest demand sectors for steel products worldwide, while the iron and steel industry accounts for about 24% of global industrial CO2 emissions [1]. In this context, improving the efficiency and rationalization of steel structural design has become increasingly important. Among these design tasks, cross-section assignment plays a key role in balancing structural performance, material use, costs, and constructability. Motivated by the growing use of graph-based methods in structural design and analysis, this paper proposes a graph-based workflow for learning structurally meaningful member groups and guiding shared cross-section assignment in steel building systems.

1.1. Structural graph representations

Recent studies related to applying graphs in structural design have increasingly developed along algorithm-centered pipelines. One major direction focuses on topology optimization, including differentiable pipelines [2, 3] and learning-based methods [4]. Related efforts have also explored conditional topology generation for structural form-finding [5]. Other studies use graph-based models to learn surrogate models for structural prediction and analysis, including beam-column frame system [6], trusses [7], and shells [8].

At the representation level, existing studies adopt either topology-derived or geometry-derived graph constructions. In topology-derived representations, structural joints are usually treated as nodes and members as edges, allowing the graph to directly encode load paths and connectivity [6, 7]. This representation is common in graph-based structural learning and optimization because it preserves the relational structure of frame or truss systems. In geometry-derived representations, the graph is instead built from finite element meshes or other geometric discretizations [4], enabling a closer connection to simulation fields and physical response quantities.

Despite these advances, most existing representations are designed primarily to support topology optimization, response prediction, or surrogate modeling, and have not been developed with member grouping and cross-section assignment in mind. In particular, no existing representation jointly encodes structural connectivity and mechanical response for the purpose of member grouping and shared cross-section assignment. This paper addresses the gap by proposing a heterogeneous graph representation that integrates both, enabling mechanics-guided grouping as a practical intermediate step in structural design.

1.2. Cross-section member selection

With a representation that captures both structural connectivity and mechanical response, the next challenge is cross-section assignment, a task where member grouping plays a central role in balancing structural performance, material use, costs, and constructability. However, determining effective groupings is difficult and often relies on designer experience, making the process time-consuming and uncertain [9]. Some studies have investigated automated optimization methods for cross-section size selection in steel structures, with the goal of achieving efficient designs while satisfying code-based constraints [10]. Nevertheless, highly optimized solutions with too many distinct member sizes may become impractical for fabrication, logistics, and on-site assembly [11]. Recent studies on cross-section selection have therefore recognized structural weight and the number of different cross-sections or member groups as conflicting objectives, and have accordingly formulated the problem within a multi-objective optimization framework [9]. Related research in computational structural design has also shown that rationalization is closely tied to reductions in manufacturing and procurement complexity, while clustering-based regularization can be used to reduce large sets of structural demands into a smaller number of representative groups [12]. More broadly, designer-driven computational workflows for structural assignment and reuse have highlighted that practical design often requires balancing structural efficiency, section rationalization, inventory or constructability constraints, and computational tractability, rather than simply pursuing the minimum possible weight [13, 14]. These studies suggest that practical cross-section selection is not merely an element-wise sizing problem, but also depends on how members are grouped and how discrete section pools are defined.

Karamba3D is a structural analysis and optimization tool for Rhino/Grasshopper that supports finite element modeling and early-stage structural design. Cross-section optimization in Karamba3D is implemented as an automated discrete sizing procedure that checks available sections within a predefined family and selects the first one satisfying the force demands of a given element, accounting for normal force, biaxial bending, torsion, and shear force [15], with beam utilization evaluated according to Eurocode 3 [16]. While it provides an efficient tool for element-wise cross-section sizing, its built-in optimizer can produce non-convergent members and overly fragmented section assignments in practice. To address these limitations, this paper proposes an unsupervised learning approach that automatically groups structural members for cross-section assignment, and then uses Karamba3D's cross-section optimization function to evaluate the resulting grouping strategies.

2. Methodology

The proposed grouping method follows a four-stage pipeline that moves from structural simulation through graph construction, embedding learning, and unsupervised clustering to arrive at grouped inputs for cross-section assignment (Fig. 1). First, we extract both topological information and mechanical-response features from the structure, where the latter are obtained through idle simulation (section 2.1). These data are then organized into a heterogeneous graph (section 2.2), in which connection points and linear members are treated as nodes, and point-line, line-point, and line-line relations are encoded as edges. Next, the heterogeneous graph is processed by a HeteroGAT model to learn an embedding for each linear member, with pairwise similarity used to guide the embedding training (section 2.3). Based on the learned embeddings, we perform unsupervised clustering using a Gaussian Mixture Model to group structurally similar members (section 2.4). The resulting clustering is finally used as grouped input for Karamba3D cross-section assignment, so that section assignment is carried out at the group level rather than independently for every member.

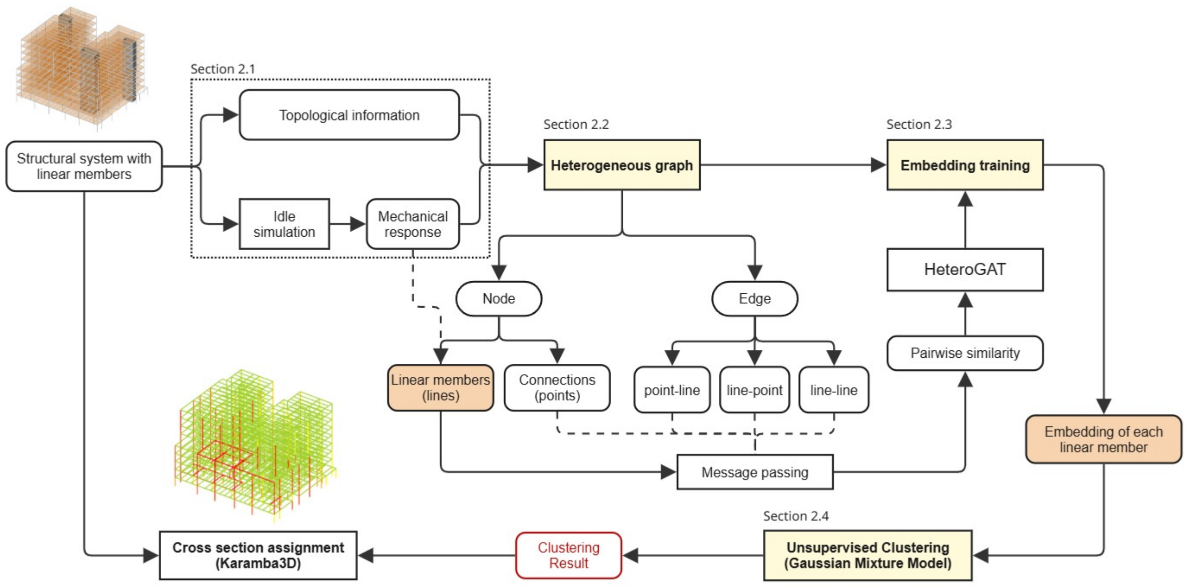

Figure 1: Overall cross-section assignment pipeline.

2.1. Idle simulation and data pre-processing

We first prepare the structural simulation data and convert it into normalized inputs for later learning. We represent the input structural system using linear members, together with the required cores and floor slabs, and assign all the linear members into three categories: columns, girders, and beams. A member is identified as a column if it spans a vertical height for more than a threshold (here set to 1.0 meter). Among the remaining horizontal members, those connected to at least one column node are labeled as girders, while the others are labeled as beams.

We perform an idle finite element analysis with Karamba3D to obtain the mechanical response, in which all members are initially assigned the same cross-section W4×13. We conduct the analysis under the following assumptions: all members are modeled as linear members; floors and cores are defined as concrete; beam-to-girder and girder-to-column connections are modeled as rotational joints about the local y-axis; and the applied loads include a dead load of 3 kN/m² based on the self-weight of the steel structural system and associated permanent components [17], a floor live load of 2 kN/m², and a roof live load of 1 kN/m² [18]. The simulation outputs a set of structural response values for each linear member, including compression, tension, shear in the z and y directions, torsional moment, and bending moments about the y and z axes. These response quantities provide the mechanical basis for later similarity learning. All node coordinates and force-related values are normalized to the range [0,1].

2.2. Heterogeneous graph construction

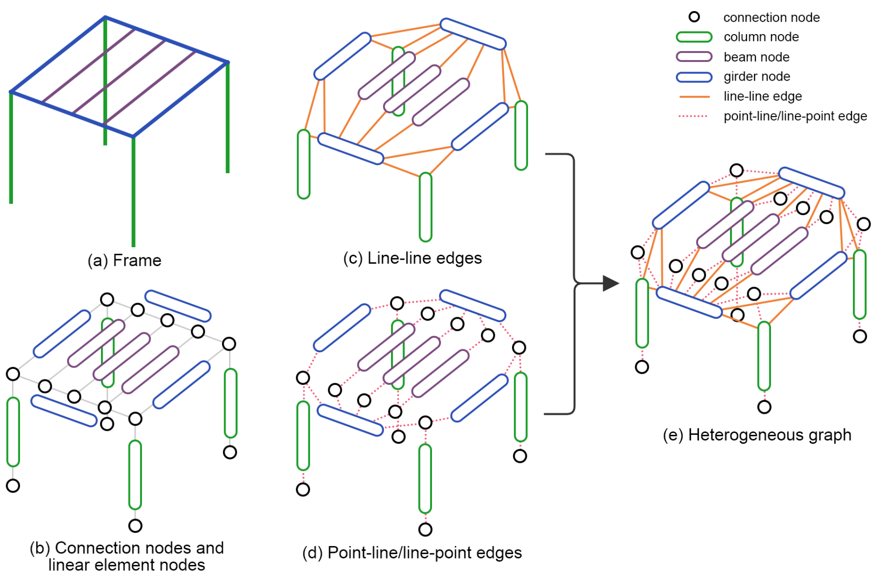

Figure 2: Heterogeneous graph representation for structural systems.

Next, we model the structure as a heterogeneous graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ (Fig.2). The graph is heterogeneous because it contains more than one type of node and relation. Specifically, the node set is defined as:

$$\mathcal{V} = \mathcal{V}_{point} \cup \mathcal{V}_{line}, \tag{1}$$

where $\mathcal{V}_{point}$ denotes the set of structural connection nodes and $\mathcal{V}_{line}$ denotes the set of linear member nodes. The heterogeneous edge set is defined as

$$\mathcal{E} = \mathcal{E}_{point\to line} \cup \mathcal{E}_{line\to point} \cup \mathcal{E}_{line\leftrightarrow line}, \tag{2}$$

where $\mathcal{E}_{point\to line}$ is the point-to-line relation, $\mathcal{E}_{line\to point}$ is the reverse line-to-point relation, and $\mathcal{E}_{line\leftrightarrow line}$ is the line-to-line adjacency relation induced by shared structural connections. We separate point-to-line and line-to-point relations because they represent two different directions of message passing, each with its own semantic role and learnable transformation. The line-line adjacency is treated as a symmetric relation, so message passing occurs in both directions between adjacent line members.

Each structural connection node $v_i \in \mathcal{V}_{point}$ is represented by a feature vector $\mathbf{x}_i$ that stores its normalized coordinates, support condition, structural degree, and shortest-path distance to the nearest support. Each linear member node $u_j \in \mathcal{V}_{line}$ is represented by a feature vector $\mathbf{x}_j$ that stores its geometric, mechanical, and topological attributes, including member length, direction, simulation-based mechanical responses, distance to support, vertical orientation, structural type, line-graph degree, and the degrees of its end nodes.

2.3. Positive pair construction and embedding training

We train an encoder to learn a vector embedding for each linear member, such that mechanically and topologically similar members are mapped to nearby points in the embedding space. To supervise this representation learning process, we construct a positive pair set

$$\mathcal{P}^{+} = \mathcal{P}^{+}_{\text{knn}} \cup \mathcal{P}^{+}_{\text{adj}}, \tag{3}$$

where $\mathcal{P}^{+}_{\text{knn}}$ denotes mechanically similar member pairs and $\mathcal{P}^{+}_{\text{adj}}$ denotes adjacency-based member pairs.

The first subset, $\mathcal{P}^{+}_{\text{knn}}$, is constructed based on mechanical similarity. For each linear member $u_i \in \mathcal{V}_{\text{line}}$, we extract a mechanical feature vector $\mathbf{m}_i$ using standardized structural response quantities, and define its positive neighbor set as the k nearest members in the mechanical feature space. k is set to 20 for experiments in this paper. The corresponding pair set is written as

$$\mathcal{N}_k^{+}(i) = \underset{\substack{\mathcal{S} \subset \mathcal{V}_{\text{line}} \setminus \{u_i\} \\ |\mathcal{S}|=k}}{\arg\min} \sum_{u_j \in \mathcal{S}} \|\mathbf{m}_i - \mathbf{m}_j\|_2 \,, \qquad \mathcal{P}^{+}_{\text{knn}} = \left\{(u_i, u_j) \mid u_j \in \mathcal{N}_k^{+}(i)\right\}. \tag{4}$$

This construction encourages the model to associate members with similar structural behavior, even if they are far apart geometrically.

The second subset, $\mathcal{P}^{+}_{\text{adj}}$, is constructed from structural adjacency. If two linear members share a structural connection, they are treated as a positive pair. This criterion is added because adjacent members often participate in related load-transfer paths and may therefore benefit from similar grouping. Formally,

$$\mathcal{P}^{+}_{\text{adj}} = \{(u_i, u_j) \mid u_i \text{ and } u_j \text{ share a structural connection}\}. \tag{5}$$

The graph encoder is a Heterogeneous Graph Attention Network (HeteroGAT) [19] with one hidden layer (dimension = 64). At each layer, the representation of node i is updated by aggregating messages from its neighbors under different relation types:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\sum_{r \in \mathcal{R}} \sum_{j \in \mathcal{N}_i^r} \alpha_{ij}^{r,(l)} \mathbf{W}_r^{(l)} \mathbf{h}_j^{(l)}\right), \tag{6}$$

where $\mathbf{h}_i^{(l)}$ denotes the feature of node i at layer l, $\mathbf{W}_r^{(l)}$ is the learnable transformation for relation type r, and $\alpha_{ij}^{r,(l)}$ is the learned attention weight.

After message passing, each linear member u_i is mapped to a low-dimensional embedding vector $\mathbf{z}_i \in \mathbb{R}^{32}$. Pairwise affinity between members is measured by cosine similarity, and the binary contrastive objective is defined as

$$s_{ij} = \tilde{\mathbf{z}}_i^{\top} \tilde{\mathbf{z}}_j, \qquad \mathcal{L} = -\sum_{(u_i,u_j) \in \mathcal{P}^+} \log \sigma(s_{ij}) - \sum_{(u_i,u_j) \in \mathcal{P}^-} \log\left(1 - \sigma(s_{ij})\right). \tag{7}$$

Here, $\mathcal{P}^+$ contains positive pairs and $\mathcal{P}^-$ contains sampled negative pairs not included in $\mathcal{P}^+$. The model is trained using Adam for 1000 epochs with a learning rate of 10^{-3}.

2.4. Structural-Type-Constrained GMM Clustering

With the vector representations from the previous section, we further cluster the linear member embeddings so that structurally similar members can be grouped together and assigned the same cross-section in the subsequent design stage. In this way, the clustering result can be used as input to the subsequent cross-section optimization process, reducing the number of independent section assignments that need to be checked and helping the optimization converge more stably. We choose Gaussian Mixture Models (GMM) [20] because they provide probabilistic clustering and can better accommodate embedding distributions with different spreads and shapes than simpler hard-assignment methods such as k-means.

After contrastive training, we cluster the learned linear member embeddings using GMM. We perform this clustering separately for each structural type, including columns, girders, and beams, since they typically carry different force demands and should therefore not be assigned to the same cross-section group solely based on embedding proximity. For each structural type t, let $\mathcal{Z}^{(t)} = \{\tilde{\mathbf{z}}_i\}$ denote the set of linear member embeddings belonging to that type. We model the distribution of embeddings within structural type t using a Gaussian Mixture Model (GMM):

$$p(\tilde{\mathbf{z}}) = \sum_{c=1}^{K_t} \pi_c^{(t)} \mathcal{N}\left(\tilde{\mathbf{z}} \mid \boldsymbol{\mu}_c^{(t)}, \boldsymbol{\Sigma}_c^{(t)}\right), \tag{8}$$

where K_t is the manually specified number of clusters for structural type t, which also determines the granularity of the final grouping for cross-section assignment; $\pi_c^{(t)}$ is the weight of cluster c, and $\mathcal{N}(\cdot)$ is a Gaussian distribution with center $\boldsymbol{\mu}_c^{(t)}$ and spread $\boldsymbol{\Sigma}_c^{(t)}$.

For each linear member embedding $\tilde{\mathbf{z}}_i$, the GMM computes how likely it is to belong to each cluster. The probability that linear member embedding i belongs to cluster c is

$$\gamma_{ic}^{(t)} = \frac{\pi_c^{(t)} \mathcal{N}\left(\tilde{\mathbf{z}}_i \mid \boldsymbol{\mu}_c^{(t)}, \boldsymbol{\Sigma}_c^{(t)}\right)}{\sum_{c'=1}^{K_t} \pi_{c'}^{(t)} \mathcal{N}\left(\tilde{\mathbf{z}}_i \mid \boldsymbol{\mu}_{c'}^{(t)}, \boldsymbol{\Sigma}_{c'}^{(t)}\right)}. \tag{9}$$

We assign each linear member to the cluster with the highest probability.

After clustering each structural type separately, we organize the final clustering output into a unified indexing system while preserving type consistency, so that the clustering can be directly mapped back to the source structural model and used as grouped input for subsequent cross-section assignment and evaluation. In the following section, this clustering strategy is evaluated on a whole-building steel structural model.

3. Results

3.1. Whole building project case study

We evaluate the proposed grouping and cross-section assignment pipeline through a whole-building steel structure case study, comparing it against both the original reference design and element-wise Karamba3D optimization, before demonstrating broader applicability to additional structural typologies. For the purposes of this analysis we use real building data from the Steel Solutions Center at the American Institute of Steel Construction, an 8-story, steel building with 11,903m2 area from Denver, Colorado, USA [21]. The structural system contains 2395 linear members in total. Consistent with the scope of the original study, only the steel gravity system was considered in the simulations and subsequent evaluation.

We compare three cross-section assignment strategies: (1) the original reference assignment from the building model, which serves as the project-specific baseline; (2) the element-wise optimization result obtained using the built-in Karamba3D cross-section optimizer, which iteratively updates member sections; and (3) the proposed clustering-based assignment generated from the learned linear-member embeddings, in which the 2395 linear members are first grouped into a total of $K = 120$ clusters using GMM before cross-section assignment. We conduct the same gravity-load condition described in Section 2.1.

In the proposed-clustering pipeline, the KNN-based embedding training (section 2.3) showed stable convergence, with the loss decreasing from 4.08 to 0.88 over 1000 epochs while the positive–negative similarity gap increased from 0.29 to 2.63, indicating progressively improved separation in the learned embedding space. The number of clusters ($K = 120$) in the GMM clustering phase (section 2.4) was selected to balance section rationalization and structural performance, and the cluster numbers for beams, columns, and girders are allocated in proportion to the number of members in each structural type. By reducing the search space from the member level to the cluster level, the proposed method only needs to check 120 groups during section selection, making convergence easier than in the element-wise case.

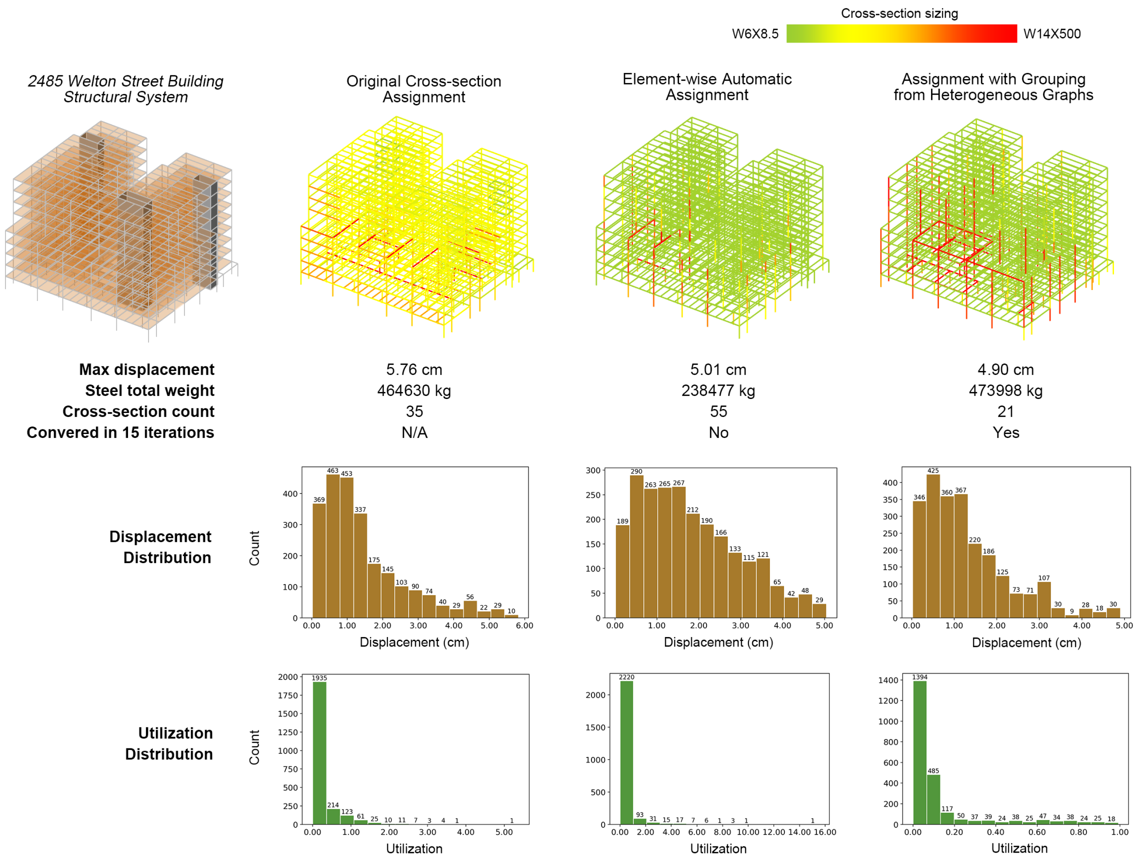

Figure 3: Comparison of cross-section distributions under the three assignment strategies.

As shown in Fig. 3, the element-wise automatic assignment achieves the lowest total steel weight and slightly reduced maximum displacement, but produces a highly fragmented solution with 55 different cross-sections and remains non-convergent even after repeated runs with increased iteration limits (from 10 to 30 iterations) in our test. By contrast, the proposed grouping-based assignment converges within 15 iterations, reduces the number of cross-sections to 21, and achieves a maximum displacement of 4.90 cm, improving upon the original reference design while remaining close to the element-wise result. The proposed method is expected to be heavier than the fully element-wise solution [9], but its total steel weight remains comparable to the original design.

The utilization histograms show that both the original design and the element-wise automatic assignment include members with utilization greater than 1.0, whereas the proposed grouped assignment keeps utilization within a safer and more controlled range. This indicates that the proposed method better maintains structural safety while reducing the complexity of cross-section assignment. Meanwhile, the displacement histograms remain relatively balanced in all three cases, suggesting that the structural response is not dominated by obvious local overstressing. Overall, the proposed automatic clustering and cross-section assignment method achieves a steel weight comparable to the original design while yielding lower maximum displacement and using the fewest cross-section types among the three strategies. Compared with element-wise cross-section optimization, it is also more stable, easier to converge, and better preserves a safe utilization range.

3.2. Broader applications

To further evaluate the proposed grouping strategy on different structural systems, we compare cluster-based assignment with element-wise assignment on a spatial truss and a gridshell, as shown in Fig. 4. In both examples, the proposed method produces a more rationalized cross-section layout and greatly reduces the number of distinct cross-sections. In addition, the grouping-based assignment leads to more stable optimization behavior and makes convergence easier. This is particularly evident in the gridshell case, where the element-wise assignment does not fully converge within the given iterations and some members remain above the utilization limit (1.0), while the proposed grouped solution achieves a more manageable and consistent section system.

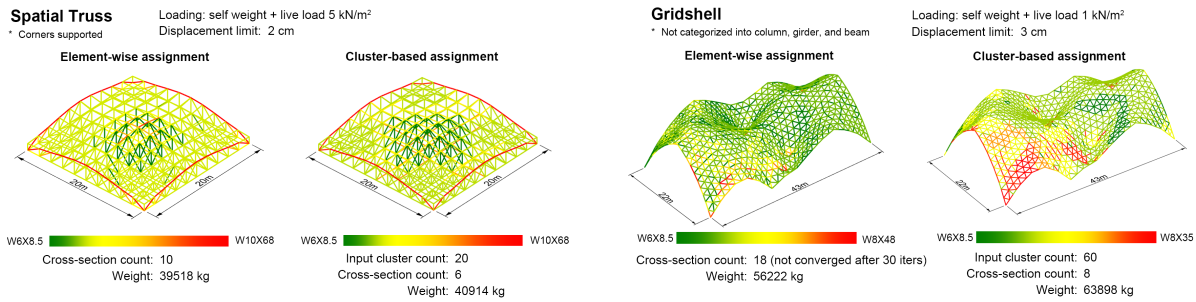

Figure 4: Cross-section assignment results of the proposed clustering method for a spatial truss and a gridshell.

4. Discussion

4.1. Representation implications

Unlike existing structural graph representations, which treat mechanical response primarily as a prediction target, the proposed heterogeneous graph encodes it directly as a feature, allowing the learned embeddings to capture behavioral similarity alongside topological context. This allows the learned embeddings to reflect not only whether members are adjacent in the structural system, but also whether they behave similarly under loading. In this sense, the representation serves as both a data structure for graph learning and as a way of organizing structural behavior to support practical design decisions such as grouping and shared cross-section assignment. Beyond the present case study, this representation may also be extended to other structural analysis, optimization, and generation tasks that require both topological and mechanical reasoning, including applications such as structural health monitoring, generative design, and multi-objective form-finding.

4.2. Cross-section optimization with clustering

From the perspective of cross-section optimization, the proposed method should not be interpreted simply as a replacement for element-wise optimization. Instead, its main contribution lies in introducing a group-aware intermediate layer between structural analysis and section assignment, which makes the overall design process more manageable, interpretable, and stable. By clustering 2395 linear members into 120 groups before optimization, the method reduces the search space from the member level to the group level, making the Karamba3D sizing process easier to converge and producing a more rationalized section system.

Although the grouped solution is heavier than the fully element-wise assignment, this is expected, since reducing the number of groups and minimizing structural weight are inherently conflicting objectives

[9]. In return, the method achieves the fewest cross-section types, keeps utilization within a safer range, and reaches a steel weight comparable to the original design with lower maximum displacement. These results suggest that the method is particularly suitable for early-stage design, where interpretability and convergence stability may be more valuable than a purely element-wise optimum.

4.3. Limitations and future work

While the proposed method demonstrates clear potential for early-stage structural design, its current form has several limitations that define the boundaries of its applicability. The most significant is that the number of clusters must be specified manually for each structural type, which requires designer judgment and makes systematic exploration across different structural systems difficult. Addressing this as a model-selection problem that jointly considers structural performance, convergence behavior, and section rationalization is the most pressing direction for future work. Additionally, the current study considers only gravity loads, following the scope of the selected case study, and future work should extend the pipeline to lateral loads and combined load combinations. Finally, the present results were obtained with a fixed set of model and training choices, including graph features, positive-pair construction, network depth, and clustering settings. A more thorough hyperparameter study may improve the quality and transferability of the learned embeddings across different structural typologies.

5. Conclusion

This paper presented a mechanics-guided grouping method for cross-section assignment in steel structural systems, combining heterogeneous graph representation learning with unsupervised clustering to support early-stage structural design. By encoding mechanical response directly as a structural feature, the method groups members according to both load-related behavior and topological context. The resulting clusters are used as grouping rules for shared cross-section assignment in Karamba3D, reducing the search space from the member level to the group level and making grouped cross-section design more feasible, stable, and rationalized than element-wise automatic sizing.

The case study shows that the method achieves the fewest cross-section types among the compared strategies, keeps member utilization within a safer range, and reaches a steel weight comparable to the original design with lower maximum displacement. More broadly, the method offers a practical way to better match loads with section groups, which can help improve the feasibility of rationalized structural design workflows in early-stage applications. Future work will extend the framework to additional load cases, develop more systematic cluster-selection strategies, and evaluate its applicability across a wider range of structural typologies.

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