Graph Type Expressivity and Transformations

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Josephine M. Thomas
GAIN - Graphs in Artificial Intelligence and Neural Networks
University of Kassel
34117 Kassel
Germany
jthomas@uni-kassel.de

Alice Moallem-Oureh
GAIN - Graphs in Artificial Intelligence and Neural Networks
University of Kassel
34117 Kassel
Germany
amoallem@uni-kassel.de

Silvia Beddar-Wiesing
GAIN - Graphs in Artificial Intelligence and Neural Networks
University of Kassel
34117 Kassel
Germany
s.bedarwiesing@uni-kassel.de

Rüdiger Nather
GAIN - Graphs in Artificial Intelligence and Neural Networks
University of Kassel
34117 Kassel
Germany
r.nather@student.uni-kassel.de

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ABSTRACT

Graph representations have gained importance in almost every scientific field, ranging from mathematics, biology, social sciences and physics to computer science. In contrast to other data formats, graphs propose the possibility to model relations between entities. Together with the continuously rising amount of available data, graphs therefore open up a wide range of modeling capabilities for theoretical and real-world problems. However, the modeling possibilities of graphs have not been fully exploited. One reason for this is that there is neither an easily comprehensible overview of graph types nor an analysis of their modeling capacities available. As a result, neither the potential of modeling with certain graph types is exhausted nor higher modeling freedom and more efficient computing of graphs after transformation to another graph type is in scope of view of many users. In order to clarify the modeling possibilities of graphs, we order the different graph types, collate their memory complexity and provide an expressivity measure on them. Furthermore, we introduce transformation algorithms between the graph types from which equal expressivity of all graph types can be inferred, i.e., they are able to represent the same information or properties respectively. Finally, we provide a guideline for the question when a graph type transformation is efficient by defining a cost function dependend on the memory complexity and the transformation runtime as a decision-making tool.

Keywords:

graph expressivity, graph representation, graph transformation, computational complexity, information encoding.

*The first three authors contributed equally.
1 Introduction

Graph-structured data has become more prominent both in theoretical and real-world problems. While certain graph types/models have been studied extensively in graph theory [7, 50] and used as models to solve combinatorial problems [28], the usage of graphs in real-world problems is a young research field despite the fact that many problems can be inherently represented as graphs. Famous examples can be found in social networks [34, 52], the power grid [44], the network of internet providers [6], citation networks [18, 46], or protein-interaction networks [29, 37], among others. Furthermore, deep learning and data analysis have recently become involved with learning on graph-structured data. Many models have been proposed for learning on different graph types which are collected in various surveys [54, 19, 25, 51]. In contrast to the learning on graphs there are disciplines which use graphs as tool for describing their research objects. For example, in automata theory and logic [33] certain formal languages can be described as finite attributed directed graphs or (infinite) trees. In addition, in mathematical linguistics specific node and/or edge attributed directed graphs can be used to describe the structure of speech parts [27].

In general, there are different types of graphs that have in common to at least contain nodes (entities) and edges (relations between the nodes), sometimes called links. Depending on the type of graph, the node and edge sets can have different properties or attributes. However, there is no overview yet of which different graph types exist and what they can model. Thus, only on a subset of graph types in combination with selected graph problems have been addressed by developed approaches so far. In addition, a lot of algorithms and models have only been developed for few graph types, e.g., graph theoretical concepts are mainly applied to (un-)directed graphs which may have additional attributes restricted to real or natural values [26]. Although there are some extensions to, e.g., hypergraphs [8] or knowledge graphs [13], many approaches are restricted to selected graph types.

Furthermore, there is currently no measure that indicates how much information a graph type can model. In particular, for modeling, e.g., real-world problems, there is no characteristic principle of which graph type can express more or less information. This leads to the fact that options for representing data in graph format are unclear. Moreover, changing the information in a graph by transforming it into another graph type requires lossless algorithms. Until now, there are only few algorithms and most of them permit losses in the information representation, as, e.g., [47, 21].

With this paper, we aim to give an insight into the diverse graph types and their expressivity as well as a guideline on the choice of a graph type for theoretical analyses or real-world applications. For this purpose, we answer the following three research questions:

(RQ1) How much information can be encoded in different graph types?
(RQ2) How computationally efficient are different graph types?
(RQ3) When and how to choose a transformation into another type?

To address the missing transparency of the existing graph types, we start with a grouped overview on graph types and their possible static and dynamic structural properties. In combination, they cover graphs used in the literature. Based on this, we give a list of their memory complexities quantified depending on the number of nodes. The memory complexities provide a worst-case statement on the computational efficiency of the different graph types (RQ2). Furthermore, we introduce an expressivity relation between graph types that indicates the amount of information a graph type can represent w.r.t. another graph type (RQ1). Additionally, it turns out that this relation is a partial order. Afterwards, we design algorithms for lossless transformations between the presented graph types and outline their worst-case runtime complexities. Together with the anti-symmetric property of the expressivity relation, the transformations constitute our main evidence that all graph types are equally expressive.

This main result leads to a higher freedom in modeling theoretical and real-world problems since all graph types can represent the same amount of information. Consequently, it remains undetermined which graph type to choose for a given problem or whether to change the type of a given graph. On the one hand, the memory complexity of the graph

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2 Graph types and graph models are used interchangeably in this paper.
types can be used as decision support to find the most profitable graph type. On the other hand, we introduce a cost function regarding the change in the memory complexity and the corresponding transformation runtime as guideline for a transformation choice.

In total, within this paper we provide the following contributions:

1. We assemble a set of **elementary graph types** (Sec. 3) and analyze their worst-case **memory complexity** (Sec. 4).
2. We introduce the concept of **graph type expressivity** (Sec. 5.1) and use it to show, that **all attributed graph types can encode the same amount of information** (Thm. 5.3). Additionally, we give important partial results to show equal expressivity also for unattributed graph types as indications for future work (Appendix A).
3. We introduce **transformation algorithms** between the presented graph types (Sec. 5.2) and evaluate their runtime complexity.
4. We define a **transformation cost-function** in Sec. 5.3 to indicate the benefits of transforming one graph type to another in terms of changing memory capacity considering the transformation runtime complexity.

2 Related Work

The topics related to this paper cover several distinct areas. On the one hand, **graphs** that serve as models for various theoretical and real-world problems are considered. On the other hand, **graph expressivity** and **graph transformations** are introduced that differ from existing expressivity usages and transformations.

**Graphs** – The concept of graphs is fundamental in the environment of discrete mathematics. Several disciplines deal with graphs from different perspectives, such as graph theory [7, 53] and algebraic graph theory [5] which work with graph properties and their relations. Furthermore, computer scientific fields like network theory [50], data mining and machine learning [9] and neural networks [45] aim to find patterns and properties in graph-structured data. Moreover, the range of graph applications are wide since graphs can model information from various domains. Starting with theoretical applications like combinatorial optimization [28], graphs also arise naturally from networks such as social networks [26], multiagent networks [35], or mobile robot networks [56], among others. In addition, several areas of natural sciences, such as chemistry [10], (computational) biology [39], medicine [58], and technical applications, e.g., novelty detection [17, 30] and manufacturing [41] profit from graph models.

**Expressivity** – The concept of expressivity plays a significant role in examining many different objects and is intended to analyze the strength of expression given to the object. For example, one of the famous expressivity results corresponds to the fact that shallow neural networks are universal approximators, i.e., any real-valued function from a wide variety of relevant function sets can be approximated arbitrarily accurately [20]. Expressivity in the context of graph neural networks (GNN) evinces the consistency of graph embeddings, i.e., how similar feature embeddings of similar graphs are. This is closely related to the Weisfeiler Lehman (WL) isomorphism test on graphs where expressiveness is measured by distinguishing structurally non-isomorphic graphs and it has been proven that most GNNs are at most as expressive as the WL-test [55, Lem. 2]. In the following, isomorphism is not taken into account since equal expressivity is utilized for graphs that exhibit the same properties.

A more similar approach to the following definition of graph type expressivity comes from linguistics and is known as language expressivity. It characterizes to which extent an ontology implements given requirements [3]. Here, the properties of graph types are utilized as requirements to defined a binary relation that indicates that one graph type is more expressive than another.

**Graph Transformations** – Motivated by different applications, there are already several transformation techniques on graph-structured data. Especially in the context of graph learning, graph embeddings provide a basis for most learning methods [23, 1]. Thus, there are many approaches that process an input graph and map it into a metric space [19]. Instead of mapping graphs into a metric space, the paper at hand focuses on transforming graphs of a specific graph type into another graph type.
There are already some established approaches for these types of transformations. Some of these approaches are rule-based, have been studied since the 1970s and have been already successfully employed in many applications \[42\]. In general, these approaches are also stricter in the sense that they consider transformations based on graph morphisms, e.g., the transformation from an attributed graph into a hypergraph \[12\], or transformations between flat and hierarchical hypergraphs \[14\].

In the context of graph games and their winning strategies the authors of \[47\] make multigraphs simple by swapping a sequence of doubled edges, i.e., any two edges \((v_1, v_2)\) and \((v_3, v_4)\) are replaced by \((v_2, v_3)\) and \((v_4, v_1)\) until no duplicates exist anymore. Nevertheless, this type of transformation is lossy due to the absence of encoding of the previous multiple edges and only re-positioning them within the new graph in a way such that they are not multiple anymore. Another more general lossy transformation is given by the graph transformations from the python package `NetworkX` \[21\] between directed and undirected graphs. Here, a directed graph is transformed into an undirected one by getting rid of the direction information of an edge and arbitrarily choosing between the attributes of the directed edges if more than one direction is available.

In this paper, however, the kind of transformations are slightly different, since the transformations are neither rule-based nor have to follow strict graph isomorphisms. Furthermore, the transformations listed here should not suffer from any loss of information.

### 3 Graphs and Graph Properties

To start with, this Section provides the foundations and defines the different elementary graph types and their possible static or dynamic structural properties.

A **graph** is a tuple of a set of nodes and a set of edges that can have various constitutions or attributes. In general, the set of nodes and edges is not further restricted, which opens up many possibilities to model with graphs. Only finite graphs are considered in the following, i.e., the node and edge sets are finite. In the following chapters up to and concluding **Definition 3.2** the focus lies on static graphs, i.e., graphs have no temporal properties. Afterward, dynamic graphs and their properties are defined.

First, a set of elementary graphs is defined from which more involved graph types can be built.

**Definition 3.1** (Static Graphs: Elementary)

1. A **directed graph** (digraph) is a tuple \(G = (\mathcal{V}, \mathcal{E})\) containing a set of nodes \(\mathcal{V} \subseteq \mathbb{N}\) and a set of directed edges given as tuples \(\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}\). The set of all digraphs is denoted as \(\mathcal{G}_d\).

2. A **(generalized) directed hypergraph** is a tuple \(G = (\mathcal{V}, \mathcal{E})\) with nodes \(\mathcal{V} \subseteq \mathbb{N}\) and hyperedges \(\mathcal{E} \subseteq \{(x, f_i) | x \in \mathcal{V}, f_i : x \rightarrow \mathbb{N}[0]\}\) that include a numbering map \(f_i\) for the \(i\)-th edge \((x, f)\), which indicates the order of the nodes in the (generalized) directed hyperedge. Wlog, it can be assumed that the numbering is gap-free, so if there exists a node \(u \in x\) with \(f(u) = k > 1\) then there will also exist a node \(v\) s.t. \(f(v) = k - 1\). The set of all (generalized) directed hypergraphs is denoted as \(\mathcal{G}_h\).

**Remark:** The definition of the generalized directed hypergraph differs from the common definition of a directed hypergraph \[8\] with edges \(\mathcal{E} \subseteq \{(x, y) | x, y \in \mathcal{V}\}\). To obtain a more generalized definition, we introduce a numbering mapping for each hyperedge that indicates an ordering of the nodes in a hyperedge. On a **generalized hyperedge** we define the ordering by equipping the node set \(x\) with a function \(f : x \rightarrow \mathbb{N}\) such that for \(u, v \in x : u \leq v \Leftrightarrow f(u) \leq f(v)\)

With this, the common notion of a directed hyperedge \((x, y)\) can be depicted by mapping the nodes in \(x\) to 1 and the nodes in \(y\) to 2. Due to this construction, not only binary relations can be considered, but also \(n\)-ary relations for arbitrary \(n\), encoding a path in a common directed hypergraph.

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3 This definition follows the one called **double edge swap** from \[40\]. It is also known as degree-preserving rewiring, checkerboard swap, tetrad or alternating rectangle \[16\].

4 `networkx.DiGraph.to_undirected`: lossy transformation, `networkx.Graph.to_directed`, lossless transformation
Another component for obtaining more graph types is to demand additional properties of the graph structure. These properties are called structural as they relate directly to the graph structure, i.e., the graph representation has to be extended or changed by further data structures.

**Definition 3.2 (Static Structural Graph Properties)**

An elementary graph $G = (V,E)$ is called

1. **undirected** if the directions of the edges are irrelevant, i.e.,
   - for directed graphs: if $(u,v) \in E$ whenever $(v,u) \in E$ for $u,v \in V$. Then an abbreviation can be the set data type instead of tuples, namely $E \subseteq \{(u,v) | u,v \in V, u \neq v\} \cup \{\{u\} | u \in V\}$. 
   - for directed hypergraphs: if $f_i : x \rightarrow 0$ for all $(x, f_i) \in E$. Abbreviated by $E \subseteq \{x | x \subseteq V\}$.

   In what follows $G_\alpha$ is the set of all undirected graphs.

2. **multigraph** if it is a multi-edge graph, i.e., the edges $E$ are defined as a multiset, a multi-node graph, i.e., the node set $V$ is a multiset, or both. All multigraphs are written as the set $G_m$.

3. **heterogeneous** if the nodes or edges can have different types (node- or edge-heterogeneous). Mathematically, the type is appended to the nodes and edges. I.e., the node set is determined by $V \subseteq \mathbb{N} \times S$ with a node type set $S$ and thus, a node $(v, s) \in V$ is given by the node $v$ itself and its type $s$. The edges can be extended by a set $R$ that describes their types, to $(e, r) \forall e \in E$ of edge type $r \in R$.

4. **attributed** if the nodes $V$ or edges $E$ are equipped with node- or edge attributes. These attributes are formally given by a node attribute function and an edge attribute function, respectively, i.e., $\alpha : V \rightarrow A$ and $\omega : E \rightarrow W$, where $A$ and $W$ are arbitrary attribute sets. In case there are only node attributes the graph is called **node-attributed**, in case of just edge attributes it is called **edge-attributed** and if we have $W \subseteq R$ it is called **weighted**. The set of all attributed graphs is denoted as $G_\alpha$.

Fig. 2 shows examples of graph types that can be obtained from elementary graphs (Def. 3.1) and additional static structural graph properties (Def. 3.2). For many theoretical as well as real-world problems, the corresponding graph model arises naturally. For example, as visualized in Fig. 2(e)], networks in which different entities or relations exist tend to be modeled in heterogeneous graphs. A simple example of this are social networks in which different groups of people exist, possibly even in different relations [11] [26]. Problems in which non-binary relations can exist, are by definition formulated as hypergraphs, as visualized in Fig. 2(b)]. See [4] for an example where the nodes of a citation network are authors and the hyperedges exist between all authors of a publication. An example are problems that contain different groupings: In the hypergraph-model, hyper-edges define different group memberships and thus connect all objects in the respective groups.

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5 the second set contains the set of self-loops
6 $f_i(x) = 0$ encodes that $x$ is an undirected hyperedge
For many mathematical problems from graph, group or number theory, simple graph structures such as (un)directed graphs are usually sufficient [28] [2] [48]. Such graphs are visualized in Fig. 2[a] and [c]. While much additional information can be encoded in attributes, there is also information that nodes or edges can more easily formulate. An example of this is the road network, where nodes represent different locations and multiple paths exist between two locations. Such problems can naturally end up in a multigraph (cf. Fig. 2[d]).

Figure 2: Visualization of the different static graph types and properties: a) directed graph, b) directed hypergraph (edges are indicated by boxes, direction by numbering), c) undirected graph, d) multigraph, e) heterogeneous graph (different relations illustrated with colors, different node types by filling), f) attributed graph.

Different to the static structural graph properties, dynamic structural graph properties include temporal dependencies. They are another component for extending to further graph types and are defined in the following.

**Definition 3.3 (Dynamic Structural Graph Properties)**

An elementary graph is called

1. **dynamic** if the graph structure or the graph properties are time depended. In the following, the notion $G_i = (V_i, E_i)$, $t_i \in T$ is used, where $T$ is a set of timestamps to emphasize the time-dependence and therefore the dynamics.

2. **growing** if it is dynamic and the node or edge sets evolve w.r.t. addition of new nodes and edges respectively. I.e., $V_i \subseteq V_{i+1}$ or $E_i \subseteq E_{i+1}$, for all $t_i \in T$.

3. **shrinking** if it is dynamic and we just allow node or edge set evolution w.r.t. deletions of nodes and edges respectively. I.e., $V_i \supseteq V_{i+1}$ or $E_i \supseteq E_{i+1}$, for all $t_i \in T$.

4. **structure-dynamic** if it is growing, shrinking or both simultaneously, i.e., in particular, the nodes $V$ or edges $E$ evolve over time due to additions or deletions of nodes or edges.

5. **attribute-dynamic** if the node or edge attribute function is time-dependent. Thus, we extend our notions of the attribute functions to $\alpha_i : V_i \rightarrow A$ and $\omega_i : E_i \rightarrow W$, for all $t_i \in T$.

6. **type-dynamic** if the graph type evolves over time. E.g., an undirected graph becomes directed from one to another time step.

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[25] also mentions splits and merges of nodes and edges. Obviously, these events are sequences of additions and deletions.
So far, new graph types are obtained by arbitrary composition of an elementary graph (Def. 3.1) and other structural properties (Def. 3.2, Def. 3.3). However, in the literature, these compositions are not always mentioned by name. For this reason, in the following, common important compositions are listed and named according to the definitions from above.

**Definition 3.4 (Combined Static Graphs)**

1. **Knowledge graphs** are defined in several ways. In [51], they are defined as heterogeneous directed graphs, while in [60] knowledge graphs are the same as heterogeneous graphs. But there are also definitions that do not see a knowledge graph as a graph, combined from the aforementioned types, see for example [15] for an overview.

2. A **multi-relational graph** [22] is an edge-heterogeneous but node-homogeneous graph.

3. A **content-associated heterogeneous graph** is a heterogeneous graph with node attributes that correspond to heterogeneous data like, e.g., attributes, text or images [57].

4. A **multiplex graph/multi-channel graph** corresponds to an edge-heterogeneous graph with self-loops [22]. Here, we have $k$ layers, where each layer consists of the same node set $V$, but different edge sets $E^{(k)}$. Additionally, inter-layer edges $\tilde{E}$ exist between the same nodes across different layers.

5. A **multiscale graph** is a multiplex graph with inter-layer edges between different nodes of differing layers [32].

6. A **spatio-temporal graph** is a multiplex graph where edges per each layer are interpreted as spatial edges and the inter-layer edges indicate temporal steps between a layer at time step $t$ and $t + 1$. They are called temporal edges [24].

**Remark:** Note that in Def. 3.4 only static combined graphs have been defined for the sake of simplicity, which does not mean that there are no dynamic combined graphs. Since the dynamic results only from additional time dependencies, one can list these as additional properties and define dynamic combined graphs. Furthermore, any static graph can be viewed from a dynamic perspective. In Sec. 5.2 we also give a simple algorithm for this (cf. Algo. 10).

**Remark:** Graphs can have further additional semantic properties like connectedness, cyclicity, scale-freeness, etc. However, these are independent from the basic graph structure. Since we consider graphs syntactically in this paper, we do not go into further graph properties that result from interpretations of the given graph structure. For further readings see [28].

After having defined elementary graph types and additional properties, the following Sections work through the research questions. For the beginning, an overview of the memory complexity of the different graph types are given in Sec. 4 that indicate their computational efficiency.

### 4 Graph Memory Complexity

Here, the memory complexity of the different graph types are used as basis for determining their computational efficiency (RQ2). The memory is represented in dependency of the number of nodes $n := |V|$ and the number of edges as a function of $n$. The memory complexity of a graph type arising from the memory needed to store its nodes and edges is denoted by $c(V, type)$ and $c(E, type)$ respectively. Tab. 1 depicts the worst-case memory complexities for different graph types.

**Remark:** Note, that the memory listed in Tab. 1 are worst-case estimations for the respective graph type for reasons of comparability. In particular, assume that all graphs are fully connected. However, if graphs are considered as a model for real-world applications, then in general, graphs will be more sparse.
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### Table 1: Worst-case memory complexities for each graph type in dependence of its number of nodes \( n \). The memories are divided into storing the nodes and edges according to the type, \( c(\mathcal{V}, \text{type}) \) and \( c(\mathcal{E}, \text{type}) \) respectively.

| Graph Type                      | Nodes \( c(\mathcal{V}, \text{type}) \) | Edges \( c(\mathcal{E}, \text{type}) \) | Total | Note                                      |
|--------------------------------|----------------------------------------|----------------------------------------|-------|-------------------------------------------|
| directed                       | \( n \)                                 | \( h \frac{N}{i} \cdot \left( \sum_{j=1}^{i} \right) \cdot j \) | \( n + \frac{h}{i} \cdot \left( \sum_{i=1}^{j} \right) \cdot j \) | \( N = 2^n - 1 \) is the maximal number of hypernodes, \( h \) is the length of the longest hyperedge and \( \{i\} \) is the appropriate Stirling number of the second kind. |
| gen. dir. hypergraph            | \( n \)                                 | \( h \cdot n \times \frac{N}{i} \cdot \left( \sum_{j=1}^{i} \right) \cdot j \) | \( \sum_{i=1}^{j} \cdot j \) | worst case fully connected               |
| undirected graph                | \( n \)                                 | \( n^2 \)                               | \( n^2 + n \) | numbering is always 0                     |
| undir. hypergraph               | \( n \)                                 | \( 2^n \)                               | \( 2^n + n \) |                                            |
| multigraph                      | \( k \cdot c(\mathcal{V}', \text{type}) \) | \( l \cdot c(\mathcal{E}', \text{type}) \) | \( k \cdot c(\mathcal{V}', \text{type}) + l \cdot c(\mathcal{E}', \text{type}) \) |                                            |
| heterogeneous                   | \( s \cdot c(\mathcal{V}, \text{type}) \) | \( r \cdot c(\mathcal{E}, \text{type}) \) | \( s \cdot c(\mathcal{V}, \text{type}) + r \cdot c(\mathcal{E}, \text{type}) \) |                                            |
| attributed                      | \( c(\alpha(\mathcal{V})) \) + c(\mathcal{V}, \text{type}) \) | \( c(\omega(\mathcal{E})) + c(\mathcal{E}, \text{type}) \) | \( c(\alpha(\mathcal{V})) + c(\mathcal{V}, \text{type}) + c(\omega(\mathcal{E})) + c(\mathcal{E}, \text{type}) \) | attribute costs \( c(\alpha(\mathcal{V})) \) + \( c(\omega(\mathcal{E})) \) contain costs for all node and edge attributes |
| structure-dynamic              | \( \sum_{i \in T} c(\mathcal{V}_i, \text{type}) \) | \( \sum_{i \in T} c(\mathcal{E}_i, \text{type}) \) | \( \sum_{i \in T} \left( c(\mathcal{V}_i, \text{type}) + c(\mathcal{E}_i, \text{type}) \right) \) | time stamp set \( T \)                     |
| attribute-dynamic              | \( T \cdot c(\alpha(\mathcal{V})) + c(\mathcal{V}, \text{type}) \) | \( T \cdot c(\omega(\mathcal{E})) + c(\mathcal{E}, \text{type}) \) | \( T \cdot c(\alpha(\mathcal{V})) + c(\mathcal{V}, \text{type}) + T \cdot c(\omega(\mathcal{E})) + c(\mathcal{E}, \text{type}) \) |                                            |
| type-dynamic                   | \( \sum_{i \in T} c(\mathcal{V}_i, \text{type}) \) | \( \sum_{i \in T} c(\mathcal{E}_i, \text{type}) \) | \( \sum_{i \in T} \left( c(\mathcal{V}_i, \text{type}) + c(\mathcal{E}_i, \text{type}) \right) \) |                                            |

**Remark:** For some of the graph types, there are already more optimized ways to store the data structure. An example of this is the use of the continuous-time dynamic representation, where one static initial graph is stored, and the subsequent snapshots are compressed in a set of events \( \mathcal{V} \) representing only the differences between two successive snapshots. As an example, this would lead to the following storage capacities, compared to those in Tab.1.
In any case, there are not enough mature graph analysis approaches for dynamic graphs like this that handle them well. Therefore, optimized graph representations are not discussed here, but only worst-case memory requirements for intuitive graph representations are considered. For further information, see [25].

As can be seen in Tab. 1, the lowest memory which is polynomial in \( n \) is required for directed and undirected graphs in the static case. In contrast, storing a generalized directed hypergraph grows highly exponentially in the number of nodes. Whenever another static graph property is included, the memory complexity either grows by a constant multiplier (see number of duplicates in a multigraph or number of node or edge types in a heterogeneous graph) or a constant factor (see maximum costs of attributes) in the worst case. These costs can grow further through considering the corresponding graph in a dynamic setting. Then, the memory is multiplied with the number of time stamps \( |T| \) which can be constant if the entire graph is already available or which may grow in the graph stream case.

5 Equal Expressivity of Attributed Graph Types

In the following, the graph type expressivity is defined to provide a comparative description of the amount of information a graph type can encode (RQ1). Afterwards, several graph type transformation algorithms are provided that are utilized to show that all attributed graph types are equally expressive.

5.1 Expressivity

Graph type expressivity is defined as a binary relation that turns out to be a partial order on the graph types. Utilizing the anti-symmetry property of partial orders, equal expressivity of all graph types is proven in Sec. 5.2.

**Definition 5.1 (Expressivity)**

A graph type \( G_2 \) is at least as expressive as a graph type \( G_1 \), if and only if \( G_2 \) encodes at least as many graph properties as \( G_1 \) denoted as \( G_1 \preceq G_2 \). In case both types encode the same graph properties it is denoted as \( G_1 \approx G_2 \).

For example, let \( G_1 \) be the set of all directed weighted graphs and \( G_2 \) the set of all undirected attributed multigraphs. Then the graph type \( G_2 \) is at least as expressive as \( G_1 \), i.e. \( G_1 \preceq G_2 \). This is justified by the fact that the graph properties of \( G_2 \) can all be modeled by graph properties of \( G_1 \): Undirected edges can be modeled by two directed edges (cf. Def. 3.2[1]), Graph weights are attributes restricted to the real numbers (cf. Def. 3.2[4]), and every set is by definition a multiset without multiple entries.

**Lemma 5.2**

The expressivity relation \( \preceq \) is a partial order, i.e., \( \preceq \) is reflexive, antisymmetric and transitive.

**Proof.**

1. **Reflexivity:** Let \( G_1 \) be a graph type. Then obviously \( G_1 \preceq G_1 \) holds.
2. **Anti-symmetry:** Let \( G_1 \) and \( G_2 \) be two graph types and \( G_1 \preceq G_2 \land G_2 \preceq G_1 \). Then, \( G_2 \) encodes at least as many graph properties as \( G_1 \) and \( G_1 \) encodes at least as many graph properties as \( G_2 \) from which follows, that they encode the same graph properties and thus are equally expressive \( G_1 \approx G_2 \).
3. **Transitivity:** Let \( G_1, G_2 \) and \( G_3 \) be graph types and \( G_1 \preceq G_2 \land G_2 \preceq G_3 \). Then, \( G_2 \) encodes at least as many graph properties as \( G_1 \) and \( G_3 \) encodes at least as many graph properties as \( G_2 \). Therefore, \( G_3 \) encodes at least as many graph properties as \( G_1 \) and thus \( G_1 \preceq G_3 \).

With the aid of the following algorithms, it is possible to make claims about the expressiveness of the different graph types which finally leads to the conclusion that all graphs are equally expressive.
5.2 Transformation Algorithms

This section discusses the graph transformations that convert a given graph from one graph type to another without loss of information. The graph type transformations can be interpreted as embedding functions from one graph type to another. In closing, it can be inferred that all discussed attributed graph types are equally expressive.

The transformation functions should fulfill two requirements. First, it should be possible to represent every graph in the new type. Second, the representation of a graph in the new type should be unique in order to prevent information loss. The first requirement indicates that the function has to be surjective, i.e., every graph in the image exists at least once. Thus, there is at least one representation of the graph in the new type. Nevertheless, the transformation has to be injective due to requirement two, i.e., it yields no more than one representation in the new graph type. Consequently, the transformation function has to be bijective.

To keep the overview of the embeddings simple, the following procedure complies: For a transformation \( f : \mathcal{G}_1 \rightarrow \mathcal{G}_2 \) of a graph type \( \mathcal{G}_1 \) to \( \mathcal{G}_2 \), only transformations of type \( \mathcal{G}_1 \) into a subset \( \mathcal{G} \subseteq \mathcal{G}_2 \) are specified. This subset corresponds to the image \( f(\mathcal{G}_1) = \mathcal{G} \) and guarantees surjectivity of \( f \) on its image. Since in the worst case the superset graph type \( \mathcal{G}_2 \supseteq f(\mathcal{G}_1) \) is not necessarily reached, a back transformation independent of \( f \) is given in the same way, which must be bijective for itself restricted to its image. With the embeddings that result from these constructions of \( f : \mathcal{G}_1 \rightarrow f(\mathcal{G}_1) \subseteq \mathcal{G}_2 \), it can be directly inferred that \( \mathcal{G}_2 \) is at least as expressive as \( \mathcal{G}_1 \). In case a back transformation is available, the same results hold for the reverse direction. Therefore, and due to Lemma 5.2, the relation \( \preceq \) induces a partial order and thus is anti-symmetric. This entails that \( \mathcal{G}_1 \) and \( \mathcal{G}_2 \) are equally expressive.

Without restriction of generality, it is assumed that all graphs of the algorithm’s domain (except for Algo. 11) are static. However, in the dynamic case, this does not pose a problem since the algorithms can be applied to the graph snapshots that occur at a fixed time. Moreover, in each case, the node and edge attribute sets are denoted as \( A \) and \( W \) and are not restricted in their data type. This is possible since attribute sets can always be extended arbitrarily, even in the dynamic case.

In the following paragraphs, lossless transformations from and between the different graph types are explained in detail. Each part includes the algorithms in pseudocode. Transformations between combined graph types are examined as well. Afterward, the expressivity relations between the different graph types are discussed.

Attributed and Unattributed Graph Types

For adding attributes to a given unattributed graph \( \mathcal{G} = (V, E) \), \( \mathcal{G} \in \mathcal{G}_{ua} \), i.e., for embedding it into the set of attributed graphs \( \mathcal{G}_a \), one natural approach is to introduce a node and an edge attribute function that assign empty attributes to the nodes and edges, as illustrated in Fig. 3. The corresponding algorithm for this procedure can be found in Algo. 1.

Since this type of embedding adds artificially empty information, it is trivially a bijection if the range of values is restricted to the image. For the expressiveness of graphs, this implies that the set of attributed graphs \( \mathcal{G}_a \) is at least as expressive as the set of unattributed graphs \( \mathcal{G}_{ua} \), i.e.,

\[
\mathcal{G}_{ua} \preceq \mathcal{G}_a.
\]

However, whether the reverse expressive power, i.e., \( \mathcal{G}_a \preceq \mathcal{G}_{ua} \), holds or not is non-trivial. Various indications (cf. Appendix §A) suggest that this direction is also valid, but the implementation is left open for future work.
Since many other transformations in the following benefit from allowing attributes, it is assumed that all graph types under consideration are attributed and only consider embeddings on attributed graphs. Alternatively, unattributed graphs can be transformed into the attributed type in linear time using Algo. 1.

Algorithm 1 Make Attributed

1: procedure MAKEATTRIBUTED(g)
2: \( \alpha : V \rightarrow A, \omega : E \rightarrow W \)
3: for all \( v \in V, e \in E \) do
4: \( \alpha(v) \leftarrow \emptyset \)
5: \( \omega(e) \leftarrow \emptyset \)
6: end for
7: return \( g' = (V, E, \alpha, \omega) \)
8: end procedure

Attributed Directed and Undirected Graph Types

Given a graph \( g = (V, E, \alpha, \omega) \) of undirected type, i.e., \( g \in \mathcal{G}_u \), the following algorithm represents an embedding into the set of directed graphs \( \mathcal{G}_d \). The idea of the algorithm is illustrated in Fig. 4. Each undirected edge in the input graph is replaced by two directed edges, one in each direction (cf. Algo. 2, line 4). To avoid losing information, each of these directed edges inherits the edge attributes of the previous undirected edges (line 5). At this point by construction, Algo. 2 is injective. If the range of Algo. 2 is restricted to its image, the algorithm is bijective. Thus, there is no information loss due to the transformation. In terms of expressivity, this kind of lossless embedding yields
\[
\mathcal{G}_u \preceq \mathcal{G}_d
\] (1)
which implies that directed graphs can encode more or equal graph properties than undirected graphs.

Algo. 3 turns a directed graph into an undirected one. The transformation encodes the graph edges’ direction into the edge attributes. In case both directions exist in the input graph, their attributes are not necessarily the same. To face this, the algorithm encodes the attributes associated with the respective directions (cf. Algo. 3, line 8). Analogous to above, injectivity is given by construction, and bijectivity follows from a restriction of the algorithms range to its image. Therefore, there is no information loss caused by the transformation, and the undirected graphs are at least as expressive as the directed ones, i.e.,
\[
\mathcal{G}_d \preceq \mathcal{G}_u
\] (2)

Figure 4: Illustration of Algo. 2 from an undirected to a directed graph via edge splitting in different directions.

Note that Algo. 2 does not require any attributes. However, since attributes are allowed after prerequisite, the back transformation that is described in Algo. 3 becomes simpler. A comparison with Algo. 12 in the appendix shows how much the algorithm benefits from allowing attributes. Algo. 3 does not describe the inverse function of Algo. 2

Nevertheless, it can also be justified that it has at least an inverse mapping since the embedding is bijective. This can best be observed in the following illustration in Fig. 5, which gets to the core of the transformation idea of Algo. 3.
Considering both embeddings and the results from the equations (1) and (2), both graph types turn out to be equally expressible, i.e.,

\[ G_u = G_d. \]  

(3)

Figure 5: Illustration of Algorithm 3 from directed to undirected graph via storing the directions and multiple attributes in the new attributes.

**Algorithm 2 Make Directed**

1. **procedure** MAKE\_DIRECTED\((g)\)  
2. \( E' \leftarrow \emptyset, \omega': E' \rightarrow \mathcal{W} \)  
3. **for all** \( \{u, v\} \in E \) **do**  
4. \( E' \leftarrow E' \cup \{(u, v), (v, u)\} \)  
5. \( \omega'((u, v)) \leftarrow (\omega((u, v)), 1) \); \( \omega'((v, u)) \leftarrow (\omega((v, u)), 1) \)  
6. **end for**  
7. **return** \( g' = \langle V, E', \alpha, \omega' \rangle \)  
8. **end procedure**

**Algorithm 3 Make Undirected**

1. **procedure** MAKE\_UNDIRECTED\((g)\)  
2. \( E' \leftarrow \emptyset, \omega': E' \rightarrow \mathcal{W} \)  
3. **for all** \( (u, v) \in E \) **do**  
4. \( E' \leftarrow E' \cup \{(u, v)\} \)  
5. **if** \( u < v \) **then** \( \Delta \) check "edge direction"  
6. \( \omega'\{(u, v)\} \leftarrow [(\omega((u, v)), 1)] \)  
7. **if** \( \exists (v, u) \in E \) **then**  
8. \( \omega'\{(u, v)\} \).APPEND\((\omega((v, u)), -1)\) \( \Delta \) append attributes of reverse direction  
9. **end if**  
10. **else**  
11. \( \omega'\{(u, v)\} \leftarrow [(\omega((u, v)), -1)] \)  
12. **end if**  
13. **end for**  
14. **return** \( g' = \langle V, E', \alpha, \omega' \rangle \)  
15. **end procedure**
Attributed Multi- and Non-Multi Graph Types

To obtain the property of multi-edges and nodes, Algo. 4 modifies an input graph \( g = (V, E, \alpha, \omega) \) without multi-nodes or edges by transforming the node and edge sets into multisets through permitting multiples (cf. Algo. 4 line 2). This procedure only changes the data type of the graph and thus is an injective function. The type of input graph is irrelevant for this algorithm, i.e., it can be an arbitrary elementary graph (cf. Def. 3.1) or can have arbitrary properties (cf. Def. 3.2, Def. 3.3).

If the algorithm is restricted to its image, it is bijective and thus a lossless transformation. As a result, the set of multigraphs \( \mathcal{G}_m \) is at least as expressive as the set of non-multigraphs \( \mathcal{G}_{nm} \), i.e.,
\[
\mathcal{G}_{nm} \preceq \mathcal{G}_m.
\] (4)

To encode the multi-edges or nodes of a multigraph \( g = (V, E, \alpha, \omega) \) in a non-multi graph, the Algo. 5 associates the duplicates of nodes and edges with the corresponding attributes and stores them as a list of attributes (cf. Algo. 5 lines 4, 5). Prior to that, the node and edge sets are transferred from multisets to sets via deleting duplicates by MAKESET (cf. Algo. 5). An example transformation can be found in Fig. 6. Since the modification of the node and edge multisets to sets without duplications is not injective, the storage of the different attributes in lines 3 to 6 guarantees the injectivity of MAKE NONMULTI. The algorithm is bijective if the range is restricted to the image and thus maintains the input information without loss. As a result, the set of non-multi graphs \( \mathcal{G}_{nm} \) is at least as expressive as the set of multigraphs \( \mathcal{G}_m \), i.e.,
\[
\mathcal{G}_m \preceq \mathcal{G}_{nm}.
\] (5)

And combining the results from equations (4) and (5) it follows that the non-multi graphs and multigraphs are equally expressive, i.e.,
\[
\mathcal{G}_{nm} \approx \mathcal{G}_m.
\] (6)

Algorithm 4 Turn into Multigraph

```
1: procedure MAKEMULTI(g)
2:     V' ← V.MAKEMULTISET, E' ← E.MAKEMULTISET ▷ transforms set into multiset
3:     return g' = (V', E', \alpha, \omega)
4: end procedure
```
Algorithm 5 Undo Multigraph

1: procedure MAKENONMULTI\(g\)
2: \(V' ← V\).MAKESET; \(E' ← E\).MAKESET \(\triangleright\) trafo. from multiset to set
3: \(\alpha' : V' → A\), \(\omega' : E' → W\) \(\triangleright\) append attrib. from node and edge duplicates
4: for all \(v ∈ V', e ∈ E'\) do
5: \(\alpha'(v) = [\alpha(w) \mid \forall w ∈ V : w = v]\)
6: \(\omega'(e) = [\omega(h) \mid \forall h ∈ E : h = e]\)
7: end for
8: return \(g\)
9: end procedure

Attributed Heterogeneous and Homogeneous Graph Types

Heterogeneous graph types can have different types of nodes or edges (cf. Def. \[3.2\][3]). For simplicity, it is assumed that they have both different node and edge types. Accordingly, the other graph types consist of exactly one node and edge type. Thus, they are called homogeneous in the literature [57]. From the definitions of these two terms, it is evident that homogeneous graph types describe a subset of the heterogeneous graph types. Hence, the transformation described by Algo.[6] is straightforward.

The idea is to introduce a node and edge type 0 and artificially extend the nodes and edges of the input graph \(g = (V, E, \alpha, \omega)\) by this type (cf. Algo.[6] line 4, 8). Clearly, this transformation also provides a bijective embedding and results in the expressivity relation

\[
G_{ hom} ≤ G_{ het}.
\] (7)

Also, the idea of the back transformation in Algo.[7] follows immediately using the attributes. The different node and edge types are encoded in an extension of the attributes, analogous to the approach in Algo.[3] where the attributes are extended by the edge directions (cf. Algo.[7] line 6, 8 and 14, 16). Fig.[7] illustrates this procedure. By construction,

Figure 7: Illustration of Algo.[7] from a heterogeneous to a homogeneous graph by encoding multiple node and edge types in the attributes and concatenating possible duplicates in the attributes.

Algo.[7] describes a bijective embedding, and therefore it comes to the expressivity relation

\[
G_{ het} ≤ G_{ hom}.
\] (8)

Since \(≤\) is anti-symmetric according to Lemma[5.2], the equations (7) and (8) result in the equal expressivity

\[
G_{ het} ≈ G_{ hom}.
\] (9)
Algorithm 6 Make Heterogeneous

1: procedure MakeHeterogeneous(\(g\))
2: \(V' \leftarrow \emptyset, E' \leftarrow \emptyset, \alpha': V' \rightarrow A, \omega': E' \rightarrow W\)
3: for all \(v \in V\) do
4: \(V' \leftarrow V' \cup \{(v, 0)\}\)
5: \(\alpha'(v, 0) \leftarrow \alpha(v)\) \>
6: end for
7: for all \(e \in E\) do
8: \(E' \leftarrow E' \cup \{(e, 0)\}\) \>
9: \(\omega'(e, 0) \leftarrow \omega(e)\) \>
10: end for
11: return \(g = (V', E', \alpha', \omega')\)
12: end procedure

Algorithm 7 Make Homogeneous

1: procedure MakeHomogeneous(\(g\))
2: \(V' \leftarrow \emptyset, E' \leftarrow \emptyset, \alpha': V' \rightarrow A, \omega': E' \rightarrow W\)
3: for all \((v, i) \in V\) do
4: if \(v \notin V'\) then
5: \(V' \leftarrow V' \cup \{v\}\)
6: \(\alpha'(v) \leftarrow (\alpha(v), i)\) \>
7: else
8: \(\alpha'(v) .\)APPEND((\(\alpha(v), i)\)) \>
9: end if
10: end for
11: for all \((e, r) \in E\) do
12: if \(e \notin E'\) then
13: \(E' \leftarrow E' \cup \{e\}\)
14: \(\omega'(e) \leftarrow (\omega(e), r)\) \>
15: else
16: \(\omega'(e) .\)APPEND((\(\omega(e), r\))\) \>
17: end if
18: end for
19: return \(g = (V', E', \alpha', \omega')\)
20: end procedure

Attributed Hyper- and Non-Hyper Graph Types

Similar to the transformations for multigraphs, there is a trivial and a non-trivial transformation algorithm for hypergraphs. By Def. 3.1, a hypergraph is a generalized version of a non-hypergraph. Consequently, the embedding of a non-hypergraph \(g = (V, E, \alpha, \omega)\) into the hypergraph type is executed in Algorithm 8 by extending the edges with a numbering function that is constantly 0. As only the numbering functions are added to the graph, that assign the value 0 to all nodes between which an edge exists (cf. Algo. 8, line 5), the bijectivity and also the expressivity relation \(G_{nh} \preceq G_h\) follow immediately.

In the reverse direction, i.e., from hypergraph type to non-hypergraph type, edges become fully connected subgraphs (cliques). If an input edge is undirected, it becomes a clique (cf. Algo. 9, lines 6-9), while a directed edge is encoded as several fully connected bipartite subgraphs, i.e., a bicliques (cf. Algo. 9, lines 11-14). The numbering, given by the numbering functions \(f_i\) from the hyperedges of the input \(g = (V, E, \alpha, \omega)\), provides the corresponding existence of the direction of an edge in the non-hypergraph (cf. Algo. 9, line 5). In particular, the numbering function is constant for nodes in undirected edges.
For better understanding, an example is visualized in Fig. 8. The blue edge containing nodes numbered all with a 0 becomes a fully connected clique. Given that the hyperedge is undirected, the non-hyperedges are directed both ways. The lowest node within this blue hyperedge also corresponds to the top node of the red hyperedge, and within this edge, the number 1 is assigned to it. This means that there must be a directed non-hyperedge from it to the lower node of the red hyperedge, which has the numbering 2. As stated in Def. (3.1) we assume wlog. that our numbering is gap-free.

Then in Algo. 9, line 5, we can observe that for all hyperedges \( e = (y, f) \) of \( g, g' \) will contain a clique for all \( k \in f(y) \), and a biclique for every \( k, k+1 \in f(y) \).

Figure 8: Illustration of Algo. 9, which transforms a hypergraph to a non-hypergraph graph. The undirected edge (blue) is turned into a fully connected subgraph (clique), while the directed edges are transformed into bicliques including the edge index in the attributes.

Due to the storage of the edge indices in lines 8 and 13, Algo. 9 is injective, and restricting the function to the image, it is also bijective. Therefore, there is no information loss, and it holds that

\[
G_h \preceq G_{nh}. \tag{11}
\]

Furthermore, it can be concluded that non-hypergraphs and hypergraphs are equally expressive, i.e.,

\[
G_{nh} \approx G_h. \tag{12}
\]

**Algorithm 8** Turn into Hypergraph

```plaintext
1: procedure MAKEHYPER(\( g \))
2: \( E' \leftarrow \emptyset \), \( \omega' : E' \rightarrow \mathcal{W} \)
3: \( i \leftarrow 0 \)
4: for all \( (u, v) \in E \) do
5: \( f_i : \{u, v\} \rightarrow \{0\}, f_i(u) \leftarrow 0, f_i(v) \leftarrow 0 \)
6: \( E' \leftarrow E' \cup \{\{u, v\}, f_i\} \)
7: \( \omega'((\{u, v\}, f_i)) \leftarrow \omega((u, v)) \)
8: \( i++ \)
9: end for
10: return \( g = (\mathcal{V}, E', \alpha, \omega') \)
11: end procedure
```
Algorithm 9 Undo Hypergraph

1: procedure MAKENONHYPER(g)
2: \( E' \leftarrow \emptyset, \omega' : E' \rightarrow W \)
3: for all \( e = (y, f) \in E \) do
4: \( \quad \text{for all} \ (u, v) \in y \times y, u \neq v \) do
5: \( \quad \quad \text{if} \ 0 \leq f(v) - f(u) \leq 1 \) then
6: \( \quad \quad \quad E' \leftarrow E' \cup \{(u, v)\} \)
7: \( \quad \quad \quad \omega'((u, v)) \leftarrow (\omega(e), i) \)
8: \( \quad \end{if} \)
9: \( \end{for} \)
10: \( \end{for} \)
11: return \( g' = (V, E', \alpha, \omega') \)
12: end procedure

Attributed Dynamic and Static Graph Types

Up to this point, the input graphs have been assumed to be static. Also, Algo. 10 takes a static graph as input and now embeds it into the set of dynamic graphs. As can be seen in Algo. 10, this is a trivial bijective embedding, since nothing is changed in the static graph \( g = (V, E, \alpha, \omega) \) itself. The temporal dependence comes from the interpretation of the graph as a static snapshot at an initial time stamp \( t_0 \). Consequently, in the context of expressivity, the set of dynamic graphs \( G_{dy} \) are at least as expressive as the set of static graphs \( G_s \), i.e.,

\[ G_s \preceq G_{dy}. \]  

While making a static graph dynamic is trivial, turning a dynamic graph into a static one is more complicated. For this direction, instead of considering the inverse mapping from the previous algorithm, which is only bijective by restricting it to its image, the following algorithm processes a dynamic graph by storing its dynamic behavior in the form of time series as attributes.

The main idea of the transformation is illustrated in Fig. 9. The graph structure from the dynamic input graph \( G = (g_1, \ldots, g_k), T = (t_1, \ldots, t_k) \) is cumulated over time, and the dynamic changes, either from the attributes or the structure, are stored in the corresponding attributes assigned with the time stamp.

![Diagram](image.png)

Figure 9: Illustration of Algo. 11 from a dynamic to a static graph by cummulating the structural information in one entire graph. The corresponding attribute time series are stored as the new attributes.

In line 2 of Algo. 11 all nodes and edges of the time stamps are collapsed and the union of these are defined as the new node and edge set. Of course, this is not yet enough for an injective embedding as required. However, this is not a problem because the unique attribute assignments in lines 3-6 directly solve this issue. By restricting the range of values of the embedding to its image, again bijectivity is obtained and hereby guarantees a transformation without any information loss. In terms of expressivity, this results in the inverse expressivity relationship

\[ G_{dy} \preceq G_s. \]  

17
Taking into account both expressivity relations \((13)\) and \((14)\) between static and dynamic graphs, equal expressivity is obtained, i.e.,

\[ G_s \approx G_{dy}, \]  

\[(15)\]

**Algorithm 10 Make Dynamic**

1. procedure **MAKE_DYNAMIC**\((g)\)
2. \(g\).RENAME\((g_{t_0})\)  \(\triangleright\) graph snapshot at time stamp \(t_0\)
3. return \(\{g_{t_0}\}\)
4. end procedure

**Algorithm 11 Make Static**

1. procedure **MAKE_STATIC**\((G)\)
2. \(V = \bigcup_{i[k]} V_i\), \(E = \bigcup_{i[k]} E_i\)
3. \(\alpha : V \rightarrow A\), \(\omega : E \rightarrow W\)
4. for all \(v \in V\), \(e \in E\) do
5. \(\alpha(v) \leftarrow [(t_i, \alpha_i(v)) ]\) \(\forall i \in [k]: v \in V_i\)
6. \(\omega(e) \leftarrow [(t_i, \omega_i(e)) ]\) \(\forall i \in [k]: e \in E_i\)
7. end for
8. return \(g = (V, E, \alpha, \omega)\)
9. end procedure

**Remark:** To the best of our knowledge, making a dynamic graph static is not common, and no publication can be found, which explicitly discusses this kind of procedure. In most cases, studying dynamic graphs is based on looking at the individual static snapshots. Another popular method for dealing with dynamic graphs is to use the resulting spatio-temporal graph introduced in Def.\(^{3.4}\). By definition, this is a static graph encoding all the temporal dependencies in their temporal edges. ◇

**Transformations between Combined Graph Types**

Up to this point, transformations have been considered that add or eliminate another structural property to a given graph of type \(G_1\); so that the graph is transformed into another graph type \(G_2\). In practice, it can happen that the graph types from and to which one intends to transform, do not only differ by one property but are somewhat further apart. In this case, a transformation between multiply combined graphs can be considered by the composition of the individual transformations defined for single structural properties that are illustrated in Fig.\(^{10}\).

Mathematically spoken, let \(G_1\) and \(G_2\) be two arbitrary (combined) graph types and \(p_i\) for all indices \(i \in [1, \ldots, j]\) the structural graph properties or a property describing an elementary graph, where \(j\) is the amount of properties that have to be changed to come from \(G_1\) to \(G_2\). Further let \(t(g, p_i)\) be the transformation to add or remove the property \(p_i\) from a graph \(g\). Then the following composition of single transformations \(t(g, p_i)\) describes one possible transformation from graph \(g \in G_1\) into the graph type \(G_2\), namely

\[ t(g, [p_1, p_2, \ldots, p_j]) = t(g, p_1) \circ t(g, p_2) \circ \cdots \circ t(g, p_j) \in G_2. \]

Note that the order within the composition of transformations is not unique. I.e., in particular, that the transformation from \(g_1 \in G_1\) to \(g_2 \in G_2\) is deterministic in the result but not in sequence. Furthermore, the order of composition directly impacts the required memory and runtime capacity, which is illustrated in the following example.

Let \(g_1\) be an unattributed directed graph and \(g_2\) an attributed undirected graph. For ease of reading, let \(A := MAKE\_ATTRIBUTED\) be the use of Algo.\(^{1}\) \(U_a := MAKE\_UNDIRECTED\) the use of Algo.\(^{3}\) where the use of attributes are allowed.
While the edge-attributes of the resulting graph $t(g_1, [A, U_a])$ are of the form $[\emptyset, \{1,-1\}^*]$ and the node-attributes are all set to be the empty set $\emptyset$, the graph $t(g_1, [U_a])$ has no node-attributes and just edge-attributes of the form $\{1,-1\}^*$. Therefore, the first transformation requires slightly more storage capacity. Of course, it is an argument that the difference is almost minimal, but this cannot always be guaranteed. Another critical point is that the single transformations of the properties are also not unique. The algorithms listed in this paper only describe a possible algorithm selection that works and can probably still be optimized in some places. In the appendix, for example, we introduce Algo. 12 which makes directed graphs undirected and does not allow any use of attributes. Replacing $U_a$ by $U :: \text{MAKEUNDIRECTEDNOTUSINGATTRIBUTES}$, i.e., considering $t(g_1, [A, U])$, results even in an almost double growth of the required memory capacity since the original graph is copied in a certain way (cf. sec. A.1).

**Expressivity of Attributed Graph Types**

In a nutshell, Fig. 11 shows that the lossless embeddings listed here result in a commutative diagram of graph type transformations. This means, in particular, that the different embeddings can be combined, and thus combined graph types can also be transformed lossless.

Note that at the very beginning of this section the condition that all the graph types $G_h$, $G_{ud}$, $G_d$ and $G_m$ are attributed has been required. With this assumption and all the expressivity relations between two graph types each, Theorem 5.3 follows directly.

**Theorem 5.3**

All attributed graph types are equally expressive.

**Proof:** Equation (15) proofs that the dynamic and static graph types are equally expressive. Since it has not been distinguished between dynamic and static in the other transformations, it is valid for both graph types that they are also equally expressive to the (un)directed type cf. Eq. (18), the multigraph type cf. Eq. (6), heterogeneous type cf. Eq. (9) and the hypergraph type cf. Eq. (12).

The above Thm. [5.3] may look unimpressive, but it carries great power. Since all attributed graph types are equally expressive, it follows that for any theoretical and real-world problem that a graph can model, any graph type can be used. The graph type does not even have to be attributed, since, by Algo. [1], it can be made attributed in linear time effort as listed in Tab. [3].

---

8Note that if a graph has just one node or edge attribute this suffices for the whole graph to be attributed.
5.3 Runtime Analysis and Transformation Cost-Function

Following the results above, the question arises of when and how to choose a graph type transformation (RQ3). In general, it is problem-specific whether a transformation is beneficial. However, a basic guideline can provide support in this decision process. For this purpose, this section defines a transformation cost function (16) that takes the input and output graph types into account, the relation of their corresponding memory capacities, and also the runtime of the transformations (cf. Tab. 2).

Let \( n = |V| \) be the number of nodes and \( m = |E| \) the number of edges in the corresponding input graph. In addition, let \( t \) be the number of time stamps of a dynamic input graph. Then, the following runtime complexities ensue.

| Algorithm             | Runtime          |
|-----------------------|------------------|
| MAKEATTRIBUTED        | \( \mathcal{O}(n + m) \) |
| MADEirected           | \( \mathcal{O}(m) \) |
| MAKEUndirected        | \( \mathcal{O}(n + m) \) |
| MAKEMulti             | \( \mathcal{O}(1) \) |
| MAKENonMulti          | \( \mathcal{O}(n^2 + m^2) \) |
| MAKEHeterogeneous     | \( \mathcal{O}(n + m) \) |
| MAKEHomogeneous       | \( \mathcal{O}(n + m) \) |
| MAKEHyper             | \( \mathcal{O}(m) \) |
| MAKENonHyper          | \( \mathcal{O}(mn^2) \) |
| MADEynamic            | \( \mathcal{O}(1) \) |
| MAKEStatic            | \( \mathcal{O}(t \cdot (n + m)) \) |

Table 2: Runtime for each graph type transformation w.r.t. \( n \) nodes, \( m \) edges and \( t \) time stamps.
To indicate whether a transformation from one graph type $G_1$ to another $G_2$ is beneficial, given the structure complexities $sc(G_1)$ and $sc(G_2)$ and the runtime $r(G_1, G_2)$ of the transformation, the upper results in Tab. 2 are merged within the following and compose the transformation cost function

$$tc(G_1, G_2) = O\left(\frac{sc(G_2)}{sc(G_1)} + r(G_1, G_2)\right).$$

As a guideline, higher values of the cost function represent less profitable transformations. Table 3 shows the results for the different selections of graph types $G_1$ and $G_2$ for the transformation cost function. The first summand $O_{sc}(\cdot)$ refers to the change in the structure complexity and the second summand $O_r(\cdot)$ refers to the worst case runtime of the transformation.

| $G_1$   | $G_2$        | $tc(G_1, G_2)$ | $tc(G_2, G_1)$ |
|---------|--------------|----------------|----------------|
| unattributed | attributed   | $O_{sc}(1) + O_r(n + m)$ | $-$            |
| undirected | directed     | $O_{sc}(2) + O_r(n + m)$ | $O_{sc}(\frac{1}{2}) + O_r(n + m)$ |
| undirected | hyper        | $O_{sc}(1) + O_r(m)$  | $O_{sc}(n^2) + O_r(mn^2)$  |
| directed  | dir. hyper   | $O_{sc}(2) + O_r(m)$  | $O_{sc}(n^2) + O_r(mm^2)$  |
| non-multi | multi        | $O_{sc}(1) + O_r(1)$  | $O_{sc}(\frac{1}{2}) + O_r(n^2 + m^2)$ |
| homogeneous | heterogeneous | $O_{sc}(1) + O_r(n + m)$ | $O_{sc}(\frac{1}{2}) + O_r(n + m)$ |
| static    | struct. dynamic | $O_{sc}(1) + O_r(1)$  | $O_{sc}(1) + O_r(k(n + m))$  |
| static    | attr. dynamic | $O_{sc}(1) + O_r(1)$  | $O_{sc}(\frac{1}{2}) + O_r(k(n + m))$  |
| static    | type dynamic | $O_{sc}(1) + O_r(1)$  | $O_{sc}(n^2) + O_r(k(n + m))$  |

Table 3: Transformation cost function evaluated for the transformations between all different graph types. $l$ is the max. number of duplicates in the input multigraph and $r$ is the number of node or edge types in the heterogeneous input graph.

Looking more closely at the results in Tab. 3, it is noticeable that they can be roughly divided into three categories. First, a category corresponds to the transformations that entail constant transformation costs. Transformations from (un-) directed to (directed) (hyper-) graph, non-multigraph to multigraph, or from static to dynamic graphs belong to this first category. These are particularly cost-effective since neither the memory requirement changes significantly, nor do the transformations require a long runtime. For these cases, one can therefore consider transformations without any doubts.

Secondly, there is a category, which covers costly transformations that involve at least quadratic effort. These include the transformations from (undirected) hypergraphs to (undirected) non-hypergraphs and from multigraphs to non-multigraphs. Especially for larger graphs, transformations of this type should be avoided and instead models that learn on the original graph type, e.g., for directed hypergraphs see [49], should be selected.

Thirdly, the remaining transformations have a medium effort. While the structural complexity is mainly reduced, a linear transformation time in the number of nodes and edges arises for the algorithms. For these transformations, a threshold has to be defined depending on the application and the given resources that restrict the choice of graph type. While for smaller graphs (low number of nodes and edges) or sparse graphs (way fewer edges than nodes), it is less costly to transform, the transformation can be prohibitively expensive for large scale data sets from, e.g., social networks [31] or similar that are often found in the literature [43].

Having introduced all transformations between different types of graphs and their transformation costs, one might wonder where the necessity of transforming graphs comes from, although the information content remains unchanged. There are both theoretical and practical reasons for this, which will be illustrated in some examples. The graph neural network model in [45] can analyze directed and undirected attributed graphs. While the authors do not discuss different types of nodes further, they emphasize the need to distinguish between coexisting edges of different types in the same data set.

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Since their model cannot be directly applied to this type of heterogeneous graph, the authors propose a solution to encode the different edge types in the edge attributes. This is pretty much equivalent to preprocessing the input graphs by applying Alg. 7. Since most graph neural networks refer to specific graph types \cite{59}, this example shows how crucial the graph type transformations are when the analysis models and the graph data are already given and are not compatible with each other.

Other examples that show how useful transformations introduced here are, come from graph theory or theoretical computer science. For example, it is well known that the so-called longest path problem is NP-hard, and the decision problem, i.e., investigating whether such a path exists at all, is NP-complete \cite{38}. Briefly formulated, it means that given an arbitrary graph, finding a simple path of maximal length in this graph takes at least non-polynomial computation time. However, it has been shown that the problem can be solved in polynomial time for directed acyclic graphs. Since most of the transformation algorithms listed here do not change the node-set and further edge information is encoded in the attributes (cf. Algo. 1, 2, 4, etc.), results on longest paths in a transformed graph can be traced back to the actual graph. An explicit example is an undirected acyclic multigraph, i.e., given an undirected acyclic multigraph $g$, the longest paths in a directed acyclic non-multigraph (after applying Algo. 2 and Algo. 5 to $g$) correspond to the longest paths in $g$.

This example shows that any graph property that remains invariant under transformations and at least one algorithm exists for a particular graph type that lies in complexity class P, there is a worthwhile transformation if the general problem lies in class NP. This is mainly because the runtimes of the transformation algorithms in this paper are all polynomial, and the composition of polynomial-time algorithms again lies in class P.

\section{Conclusion}

This paper aimed to motivate the usage of diverse and suitable graph types as a model for real-world problems and theoretical graph analyses. This has led to three research questions that we addressed in this paper: how much information can different graph types encode, how efficient is their use measured by the required memory complexity, and under which circumstances is a transformation from one graph type to another practically useful?

To ensure a solid basis for answering the research questions, a comprehensive overview of graph types and their properties has been presented in Sec. 3. Especially, the focus has been on graphs from scientific disciplines where they serve as models for a variety of problems. In general, the graph types result from extensions of elementary graphs by static or dynamic properties. Among the commonly used graph types in the literature, two new graph types have been presented, namely a generalization of the directed hypergraph (Def. 3.1) and the type-dynamic graph (Def. 3.3).

Furthermore, to investigate the first research question on how much information each graph type can encode, the concept of expressivity has been introduced (Sec. 5.1). It relates the different graph types to each other depending on how many properties they are able to encode. Lem. 5.2 has proved that this relation is a partial order on the graph types, which serves as one of the arguments to show in Thm. 5.3 that all attributed graph types are equally expressive. Another significant result for this inference has been the lossless transformations from one graph type to another, presented in Sec. 5.2. These transformations resemble bijective embeddings from one graph type into another under which the graph information remains invariant. In App. A partial results are listed to show additionally equal expressivity for unattributed graph types as an indication for future work. However, much graph data is attributed or can easily be attributed due to Alg. 1. Considering the equal expressivity of all attributed graph types, the reader of this paper can therefore choose a graph model based on efficiency. Additionally, the varying structures and properties of graphs can contribute to a better understanding of the information and the model behaviour. Hence, selecting different graph types for the modeling process may support, e.g., explainability of learning models on graphs.

\footnote{Acyclic graphs do not contain any paths that create circles.}
Finally, to answer the third question, if and which graph type transformation is practically useful, a transformation cost function has been defined in Sec. 5.3. The cost function respects the runtime of the algorithms per se (Tab. 2) and the memory complexities of each graph type (Tab. 1), resulting from the answer to the second research question in Sec. 4.

To conclude, due to the plurality and complexity of different graph learning problems or graph analyses, it is not possible to give a general statement about if a graph type transformation should be applied or not. However, there are some tools that can be helpful in such a decision based on computational capacities and available algorithmic tools. Apart from that, the paper implies that due to the equal expressiveness of the different graph types and the lossless transformations listed here, each graph type is equally suitable for each problem if only the information encoded in the model is considered. Computational efficiency can additionally be regarded by taking the transformation cost function into account. Besides, a graph can be transformed with the given algorithms into another type without loss, e.g., if it is known that a different graph type is advantageous. Based on this, a variety of new graph analysis methods on less common graph types can be used, and with this, many solutions to real-world problems can be solved in the future.

Notation

Throughout the paper we will use the following notation.

| Symbol | Description |
|--------|-------------|
| $\mathbb{N}$ | natural numbers |
| $\mathbb{N}_0$ | natural numbers starting at 0 |
| $\lfloor \cdot \rceil$ | absolute value |
| $[n], n \in \mathbb{N}$ | sequence $1, 2, \ldots, n$ |
| $[n], n \in \mathbb{N}_0$ | sequence $0, 1, \ldots, n$ |
| $\emptyset$ | empty set |
| $\{\cdot\}$ | set |
| $\{\cdot\}^*$ | tuple of arbitrary length over $\{\cdot\}$ |
| $\{|\cdot|\}$ | multiset, i.e. set allowing multiple appearances of entries |
| $P(\cdot)$ | power (multi)set |
| $\wedge$ | conjunction |
| $\cup$ | union of two (multi)sets |
| $\uplus$ | disjoint union of two (multi)sets |
| $\subseteq$ | sub(multi)set |
| $\subset$ | proper sub(multi)set |
| $\times$ | factor set of two sets |
| $[\cdot, \ldots, \cdot]$ | listing |
| $[\cdot, \ldots, |\cdot|]$ | list comprehension |

Table 4: Notation table

Contributions

The first three authors contributed equally. Rüdiger Nather contributed the definition of a (generalized) directed hypergraph in 3.1 and helped to improve the proofs in Section 5.1 by proofreading and comments.
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A Appendix: Equal Expressivity for Unattributed Graphs

In the following, three partial results are presented that indicate that Thm. 5.3 could also apply to the unattributed graphs occurring here. The results are called partial due to the fact that corresponding requirements have to be provided by the resulting graph type that can encode the attributes. I.e., in particular, the following transformations are discussed:

- In Sec. A.1 unattributed directed and undirected graphs are proven to be equally expressive. Nevertheless, in comparison to Algo. 3 the following algorithm requires for the additional storage of a copy of the nodes.
- Sec. A.2 illustrates an algorithm of the encoding of edge weights in the graph structure of an unattributed multigraph. The corresponding Algo. 13 uses the permission of storing duplicates to encode natural weights in the structure.
- In Sec. A.3 the idea of encoding attributes in form of different node- and edge types in a heterogeneous graph is described. Thus, the heterogeneity of the output graph type is required.

A.1 Unattributed Directed and Undirected Graph Types

The transformation from the undirected graph type to the directed graph type is described in Algo. 2 and does not require attributes at any point. Provided that the reverse direction or the transformation from the directed to the undirected graph type also does not require any attributes, a higher memory requirement arises in the transformation algorithm Algo. 12 itself. While Algo. 3 encodes the directions of the edges in the allowed edge attributes, the directions of the edges must result directly from the graph structure itself.

Note that this algorithm does not describe the inverse function of Algo. 2. Nevertheless, it can also be justified that it has at least an inverse mapping, since the embedding is bijective. This can best be observed in the following illustration in Fig. 12 which gets to the core of the transformation idea of Algo. 3.

![Illustration of Algorithm 3 from directed to undirected graph via edge decomposition method.](image)

The main idea behind the embedding is first to decompose the edge set into two sets of edges of different directions. Mathematically, the individual directions are determined by the order on the indices in the edges (Algo. 3 line 8). This means in particular, the new edge set is given by the disjoint union

$$E' = \{ (u, v) \mid u < v \} \cup \{ (v', u') \mid u \geq v \}.$$ 

Each subset describes one direction and induces one undirected graph component.

Formally, however, this is a single graph that has two subgraphs that are not connected. While the nodes of the input graph are used for one subgraph, i.e., for one direction, a copy of the nodes encodes the other direction in the other subgraph (cf. Algo. 3 line 3). Additionally, the node and edge attributes of the new graph are taken from the initial graph (cf. Algo. 3 lines 5, 10, 13). This construction guarantees the algorithm to be injective.
With a restriction of the range of Algo. 3 to its image the algorithm is bijective and there is no information loss. In terms of expressivity this kind of lossless embedding yields to

\[ G_{ad} \preceq G_{a\bar{u}}. \]  

(17)

Considering both embeddings, i.e. Algo. 2 and Algo. 3 and the results from the equations (1) and (17), both graph types turn out to be equally expressive, i.e.,

\[ G_{a\bar{u}} \approx G_{\bar{a}d}. \]  

(18)

Algorithm 12 Make Undirected

1: *procedure* MAKEUNDIRECTED\((g)\)
2: \(E' \leftarrow \emptyset\)
3: \(V' \leftarrow V \cup \{v.RENAME(v') \mid v \in V\}\) ◄ double the node set
4: *for all* \(v' \in V'\) *do* ◄ copy the node attributes
5: \(\alpha'(v') = \alpha(v)\)
6: *end for*
7: *for all* \((u, v) \in E\) *do* ◄ insert undirected edges
8: *if* \(u < v\) *then* ◄ forward edges stay between original nodes
9: \(E' \leftarrow E' \cup \{\{u, v\}\}\)
10: \(\omega'((u, v)) = \omega((u, v))\)
11: *else* ◄ backwards edges are set between new nodes
12: \(E' \leftarrow E' \cup \{\{v', u'\}\}\)
13: \(\omega'((v', u')) = \omega((u, v))\)
14: *end if*
15: *end for*
16: *return* \(g' = (V', E', \alpha', \omega')\)
17: *end procedure*

A.2 Integer Attributed Graph Types and Unweighted Multigraphs

Restricting the attributes from Def. 3.2 to natural numbers incl. zero, the following algorithm encodes the attributes in a corresponding number of duplicates of the edges. Since Algo. 1 already provided a transformation for unattributed to attributed graphs, only the reverse direction is given in Algo. 13.

Considering the natural numbers in the attributes as count of duplicates of the nodes and edges, the algorithm is obviously injective. Together with Algo. 5 as inverse function, the algorithm is bijective and the set of multigraph types is at least as expressive as the set of integer attributed graph types \(G_{ia}\), i.e.,

\[ G_{ia} \preceq G_{a\bar{m}}. \]  

(19)

It can be directly seen that the set of attributed graphs \(G_a\) is at least as expressive as \(G_{ia}\) since the attributes are restricted. Thus, together with Algo. 1 it can be concluded that both sets are equally expressive:

\[ G_{a\bar{u}} \approx G_{a\bar{m}}. \]  

(20)
Algorithm 13 Make Unattributed using duplicates

1: procedure \textsc{MakeUnattributedMulti}(g)
2: \hspace{1em} \mathcal{V}' = \emptyset.\textsc{makeMulti}, \mathcal{E}' = \emptyset.\textsc{makeMulti} \triangleright\text{introduce node- and edge- multisets}
3: \hspace{1em} for all \ v \in \mathcal{V}, e \in \mathcal{E} do
4: \hspace{2em} \mathcal{V}'.\textsc{addKTimes}(v, \alpha(v)) \triangleright\text{add } \alpha(v) \text{ duplicates of } v \text{ to } \mathcal{V}'
5: \hspace{2em} \mathcal{E}'.\textsc{addKTimes}(e, \omega(e)) \triangleright\text{add } \omega(e) \text{ duplicates of } e \text{ to } \mathcal{E}'
6: \hspace{1em} end for
7: return \(g' = (\mathcal{V}', \mathcal{E}')\)
8: end procedure

A.3 Attributed to Heterogeneous Graphs

Another idea for encoding attributes in the structure of a graph type is to introduce one node type for each unique node attribute and one edge type for each unique edge attribute. Then, the output graph is assumed to be heterogeneous, and each node or edge is of the type of its origin attribute, respectively. Algo. [14] defines the disjoint different types by using the attributes and with this builds the unattributed heterogeneous graph.

Assuming that the \textit{type} operator is bijective by assigning a different type to each unique attribute, Algo. [14] is injective and again restricting it to its image, the algorithm becomes bijective, and the unattributed heterogeneous graph types \(G_{ah}\) are at least as expressive as the attributed graph types:

\[
\mathcal{G}_a \preceq \mathcal{G}_{ah}. \tag{21}
\]

Combining (21) and Thm. [5,3] it follows that

\[
\mathcal{G}_a \cong \mathcal{G}_{ah}. \tag{22}
\]

Algorithm 14 Make Unattributed with the aid of heterogeneity

1: procedure \textsc{MakeUnattributedHeterogeneous}(g)
2: \hspace{1em} \mathcal{V}' = \emptyset, \mathcal{E}' = \emptyset
3: \hspace{1em} for all \ v \in \mathcal{V}, e \in \mathcal{E} do
4: \hspace{2em} \mathcal{V}' \leftarrow \mathcal{V}' \cup (v, \text{type}\alpha(v))) \triangleright\text{add } v \text{ with type } \text{type}(\alpha(v)) \text{ to } \mathcal{V}'
5: \hspace{2em} \mathcal{E}' \leftarrow \mathcal{E}' \cup (e, \text{type}\omega(e))) \triangleright\text{add } e \text{ with type } \text{type}(\omega(e)) \text{ to } \mathcal{E}'
6: \hspace{1em} end for
7: return \(g' = (\mathcal{V}', \mathcal{E}')\)
8: end procedure