Ubergraphs: A Definition of a Recursive Hypergraph Structure

Cliff Joslyn, Kathleen Nowak

1 Introduction

Partly in service of exploring the formal basis for Georgetown University’s AvesTerra database structure, we formalize a recursive hypergraph data structure, which we call an ubergraph. This type of data structure has been alluded to in passing but no formal explication exists to our knowledge. As hypergraphs generalize graphs by allowing edges to have more than two vertices, ubergraphs generalize hypergraphs by allowing edges to contain other edges as vertices. Thus, all graphs are hypergraphs and all hypergraphs are ubergraphs.

The ability to do indirection in graph data structures by “quoting” or “pointing to” edges is absolutely central in graph-based data science, and is accomplished in such systems by a variety of ad hoc mechanisms such as reification. Hypergraphs are frequently used as part of that armamentarium, but ubergraphs are a more robust representation framework.

Note that here we deal only with undirected hyper- and ubergraphs. Direction and/or orientation could prove very valuable, but await further consideration [2].

2 Hypergraphs

A hypergraph is a generalization of a graph in which an edge can connect any number of vertices.

Definition 1. A hypergraph \( H \) is a pair \((V, E)\) where \( V \) is a set of vertices and \( E \subseteq \mathcal{P}(V) \) is a set of non-empty subsets of \( V \). The elements of \( E \) are called hyperedges.

\[1^\text{https://en.wikipedia.org/wiki/Hypergraph#Generalizations} \]
Note 1. An abstract simplicial complex is a hypergraph whose edge set is closed under subset.

The incidence matrix and Levi graph of a (hyper)graph express vertex-edge membership.

Definition 2. Let $H = (V, E)$ be a hypergraph with $|V| = n$ and $|E| = m$. The incidence matrix of $H$ is the $n \times m$ matrix $M$ defined by

$$M_{ij} = \begin{cases} 1 & \text{if } v_i \in e_j \\ 0 & \text{otherwise.} \end{cases}$$

Definition 3. Let $H = (V, E)$ be a hypergraph with $|V| = n$ and $|E| = m$. Then the Levi graph is the bipartite graph $G = (V \cup E, E')$, where $(v_i, e_j) \in E'$ if and only if $v_i \in e_j$.

Example 1. Let $H$ be the hypergraph with vertex set $V = \{1, 2, 3, 4, 5\}$ and edge set

$$E = \{\{1\}, \{1, 3\}, \{2, 3\}, \{1, 3, 5\}\}.$$

The incidence matrix for $H$ is

$$M = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

and the Levi graph representation is

Where the Levi graph represents the vertex-edge membership relation $\in$, since $E \subseteq \mathcal{P}(V)$ is a set system of $V$, it also manifests edge-edge inclusion as a partial order on the edges through $\subseteq$. This can also be read from the Levi graph as $N^-(e_i) \subseteq N^-(e_j)$ if and only if $e_i \subseteq e_j$. In our example, we have $e_1 \subseteq e_2 \subseteq e_4$, while $e_3$ is non-comparable.
3 Ubergraphs

One way to generalize hypergraphs is to allow edges to contain not only vertices but other edges. For a finite set \( X \), we define

\[
P(X)^k = \mathcal{P} \left( \bigcup_{i=0}^{k} P_i \right), \quad \text{where } P_0 = X \text{ and } P_i = \mathcal{P} \left( \bigcup_{j=0}^{i-1} P_j \right) \text{ for } i \geq 1.
\]

**Definition 4.** A depth \( k \) ubergraph \( U \) is a pair \((V, E)\) where \( V \) is a set of fundamental vertices and \( E \subseteq \mathcal{P}(V)^k \) is a finite set of uberedges. Additionally, if \( s \notin V \) belongs to an edge, we require that \( s \) is itself an edge.

**Note 2.** Every hypergraph is a depth 0 ubergraph.

Since uberedges are allowed to contain other edges, we call the elements of \( V \cup \left( \bigcup_{e \in E} e \right) \) vertices and the elements of \( V \) fundamental vertices.

Let \( U = (V, E) \) be an ubergraph with \( |V| = n \) and \( |E| = m \). The incidence matrix of this type of hypergraph is a matrix \( M \) of order \((n + m) \times m\) where

\[
M_{xy} = \begin{cases} 
1 & \text{if } x \in y \\
0 & \text{otherwise.}
\end{cases}
\]

Moreover, the Levi graph of a hypergraph generalizes to what we will call the uber-Levi graph of \( U \) to express uberedge membership. It has one vertex corresponding to each fundamental vertex and edge of \( U \) and a directed edge from \( x \) to \( y \) if \( x \) is a member of \( y \) in \( U \).

**Example 2.** Let \( U \) be the ubergraph with fundamental vertex set \( V = \{1, 2, 3\} \) and edges

\[
E = \{e_1, e_2, e_3, e_4, e_5\} = \{\{1\}, \{1, 3\}, \{1, 3, e_1\}, \{2, e_2\}, \{1, e_4\}\}
\]

\[
= \{\{1\}, \{1, 3\}, \{1, 3, \{1\}\}, \{2, \{1, 3\}\}, \{1, \{2, \{1, 3\}\}\}\}
\]
The incidence matrix for $H$ is

$$M = \begin{bmatrix}
1 & 1 & 1 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 \\
0 & 1 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

and the uber-Levi graph representation is

Note 3. The uber-Levi graph is a directed acyclic graph (DAG). The roots (vertices with no in-neighbors) correspond to the fundamental vertices of $U$, and the vertices with positive in degree correspond to the edges of $U$. Moreover, every DAG yields an ubergaph.

Where the uber-Levi graph represents the vertex-edge membership relation $\in$, since $E \subseteq \mathcal{P}(\bigcup_{i=0}^{\infty} P_i)$ is a set system of $\bigcup_{i=0}^{\infty} P_i$, it also manifests edge-edge inclusion as a partial order on the edges through $\subseteq$. As before, this can be read from the uber-Levi graph since $e_i \subset e_j$ if and only if $N^-(e_i) \subset N^-(e_j)$. In our example, we have $e_1 \subset e_2 \subset e_3$ and $e_1 \subset e_5$, while $e_4$ is non-comparable.
As constructed so far, ubergraphs can express the syntax of generalized graph data structures like AvesTerra, where nodes can have a variable number of attributes, and in turn those attributes can be other nodes. In our example, we have $e_1 \in e_3$: the uberedge $e_3$ has another uberedge $e_1$ as an element.

Additionally, it has been discussed that AvesTerra may wish to model situations where edges can refer to themselves, either directly or indirectly. This corresponds to dropping the requirement: If $s \in P_i, i > 0$, belongs to an edge, then $s$ is itself an edge. In our example, if we were to change the definition of $e_5$ from $e_5 = \{1, e_4\}$ to $e'_5 = \{1, e_4, e_2\}$, then the uber-Levi graph would change to

\[ U = (V,E) \]

Note the inclusion of a cycle, making the uber-Levi graph now a general directed graph. Allowing (ultimately) expressions like $e = \{e\}$, and thus arbitrary cycles in the uber-Levi graph, violates the axiom of foundation. The vertex set is no longer well defined, and non-well-founded sets would need to be invoked.

### 3.1 Basic Concepts

Ubergraphs are a generalization of hypergraphs, hence many of the definitions of hypergraphs carry verbatim to ubergraphs. Most of the vocabulary given here is generalized from $[1]$.

Let $U = (V,E)$ be a depth $k$ ubergraph with $|V| = n$ and $|E| = m$. Let $M$ be the incidence matrix of $U$. By definition the empty ubergraph has
$V = E = \emptyset$ and we call any ubergraph with $V \neq \emptyset$ and $E = \emptyset$ a *trivial ubergraph*. For $e \in E$, we define

$$V^0(e) = \bigcap_{S \subseteq V, e \subseteq P(S)^k} S$$

to be the minimum set of fundamental vertices in an ubergraph containing $e$. Then we have the following analogs of subgraph:

- For $E' \subseteq E$, the ubergraph $(V, E')$ is called a *sububergraph*.
- For $V' \subseteq V$, the *induced sububergraph* $U[V']$ of the ubergraph $U$ is the ubergraph $U(V') = (V', E')$ where

$$E' = \{ e \in E \mid V^0(e) \subseteq V' \}.$$

Let $U$ be the ubergraph with vertices $V = \{1, 2, 3, 4, 5\}$ and edge set

$$E = \{ \{1, 2\}, \{1, \{1, 2\}\}, \{3\}, \{\{1, 4\}\}, \{1, 4, 5\} \}.$$

Then $U' = (\{1, 2, 3, 4, 5\}, \{\{1, 2\}, \{1, 4, 5\}\})$ is a sububergraph of $U$ and $U[\{1, 2\}] = (\{1, 2\}, \{\{1, 2\}, \{1, \{1, 2\}\}\})$.

Two vertices $x, y$ of an ubergraph are *adjacent* if there is an uberedge which contains both elements. Two uberedges are *incident* if their intersection is not empty. The *degree* of a vertex $x$ is the number of uberedges containing $x$.

Let $x, y \in V \cup E$. A *path* $P$ from $x$ to $y$ is a sequence

$$x = x_1, e_1, x_2, e_2, \ldots, x_s, e_s, x_{s+1} = y$$

such that

- $x_1, x_2, \ldots, x_{s+1}$ are all distinct vertices except possibly $x_1 = x_{s+1}$,
- $e_1, e_2, \ldots, e_s$ are distinct uberedges, and
- $x_i, x_{i+1} \in e_i$ for all $i = 1, 2, \ldots, s$.

If $x = y$ the path is called a *cycle*. The integer $s$ is the *length* of the path. We say that $U$ is *connected* if for every pair of vertices, there is a path which connects these vertices; otherwise we describe $U$ as *disconnected*. 
3.2 Matrices, Ubergraphs, and Entropy

Let $U = (V,E)$ be an ubergraph with $|V| = n$ and $|E| = m$. As stated earlier, the incidence matrix of an ubergraph is an $(n + m) \times m$ matrix $M$ where

$$M_{xy} = \begin{cases} 1 & \text{if } x \in y \\ 0 & \text{otherwise.} \end{cases}$$

Many basic concepts can be computed from the incidence matrix. For example, the degree of a vertex $x$ is $(M1)_x$ and two uberedges are incident if and only if the inner product of the corresponding rows of $M$ is nonzero.

Further, the incidence matrix of any (induced) sububergraph is a submatrix of $M$.

Next, we define the adjacency matrix $A(U)$ of $U$ to be the square matrix whose rows and columns are indexed by the fundamental vertices and edges of $U$ such that for all $x,y \in V \cup E$,

$$A_{xy} = \begin{cases} |\{e \in E \mid x,y \in e\}| & \text{if } x \neq y \\ 0 & \text{otherwise.} \end{cases}$$

Let $D(x) = \sum_{y \in V \cup E} a_{x,y}$. Then the Laplacian matrix of $U$ is given as

$$L(U) = D - A(U)$$

where $D = diag(D(v_1), \ldots, D(v_n), D(e_1), \ldots, D(e_m))$. Note that $L(U)$ is Hermitian so its eigenvalues are real. Further, by an application of the Gershgorin disk Theorem, they must be nonnegative. Since $\sum_{i=1}^{n+m} \lambda_i = Tr(L(U)) = \sum_{i=1}^{n+m} D(x_i) := \hat{d}$, we have that

$$(\mu_i)_{i=1}^{n+m} := \left(\frac{\lambda_i}{\hat{d}}\right)_{i=1}^{n+m}$$

is a discrete probability distribution. Thus, we can define the algebraic ubergraph entropy of $U$ by

$$I(U) = - \sum_{i=1}^{n+1} \mu_i \log_2(\mu_i).$$
3.3 Similarity and Metric on Ubergraphs

When we have two structures, one of the most important tasks is to compare them. This comparison is done with an isomorphism.

Definition 5. Let \( U = (V, E) \) and \( U' = (V', E') \) be two ubergraphs. We say that \( U \) and \( U' \) are isomorphic, denoted \( U \cong U' \), if there exists a bijection \( \varphi : V \to V' \) such that

\[
e \in E \text{ if and only if } \varphi(e) := \{ \varphi(x) \mid x \in e \} \in E'.
\]

This similarity measure is manifested in both the uber-Levi graph and the incidence matrix.

Theorem 1. Two ubergraphs are isomorphic if and only if their uber-Levi graphs are isomorphic.

Proof. Let \( U \) and \( U' \) be ubergraphs with uber-Levi graphs \( D \) and \( D' \) respectively. First suppose that \( U \cong U' \) and let \( \varphi : V(U) \to V(U') \) be an isomorphism. Define

\[
\psi : V(D) \to V(D') \text{ by } \psi(v) = \varphi(v) \text{ and } \psi(e) = \varphi(e) = \{ \varphi(x) \mid x \in e \}.
\]

Then

\[
(x, y) \in E(D) \overset{def}{\iff} x \in y \overset{\varphi}{\Rightarrow} \psi(x) \in \psi(y) \overset{def}{\iff} (\psi(x), \psi(y)) \in E(D').
\]

Now suppose that \( D \cong D' \) and let \( \psi : V(D) \to V(D') \) be an isomorphism. We claim that \( \psi|_{V(U)} \) is an isomorphism from \( U \) to \( U' \). First note that \( v \) is a fundamental vertex if and only if it’s in-degree in the uber-Levi graph representation is zero. Thus, since isomorphisms preserve degree, we must have that \( \psi|_{V(U)} \) is bijection from \( V(U) \) to \( V(U') \). Further,

\[
x \in e \overset{def}{\iff} (x, e) \in E(D) \overset{\varphi}{\Rightarrow} (\psi(x), \psi(e)) \in E(D') \overset{def}{\iff} \psi(x) \in \psi(e).
\]

Thus, by recursively applying this argument we have that \( \psi|_{V(U)} \) is a bijection from \( V(U) \) to \( V(U') \) such that \( e \in E(U) \) if and only if \( \psi|_{V(U)}(e) \in E(U') \). □
References

[1] "Alain Bretto". "Hypergraph Theory". "Springer International Publishing", "2013".

[2] "Giorgio Gallo, Giustino Longo, and Stefano Pallottino". "directed hypergraphs and applications". "Discrete Applied Mathematics", "42"."177–201", "1993".