DiHypergraphs

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Overview

1. Dihypergraphs

2. Species/Reaction Digraphs

3. Thanks for your attention!!!

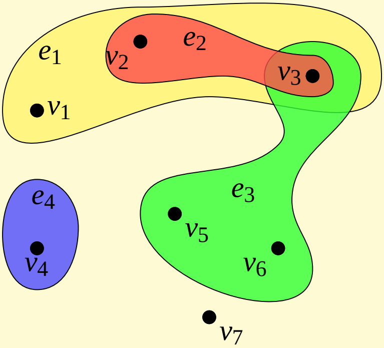
Dihypergraphs

Definition

A *(weighted) hypergraph* $H = (V(H), E(H))$ consists of a:

- *vertex set* $V(H)$: a set of elements, called *vertices*
- *edge set* $E(H)$: a set of (multi)sets on $V(H)$

Example

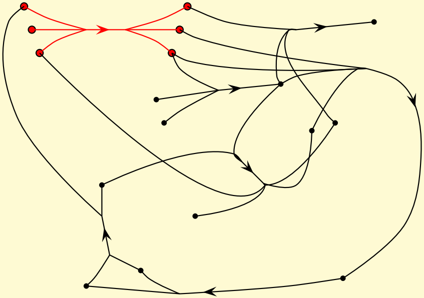


Definition

A *directed hypergraph / dihypergraph* H is $(V(H), \mathcal{E}(H))$ where:

- $V(H)$ is a set of elements, called *vertices*
- $\mathcal{E}(H)$ is a set of ordered pairs $e = (t(e), h(e))$ of (multi)sets $t(e), h(e)$ on $V(H)$, called *hyperarcs / reactions*
-

Example



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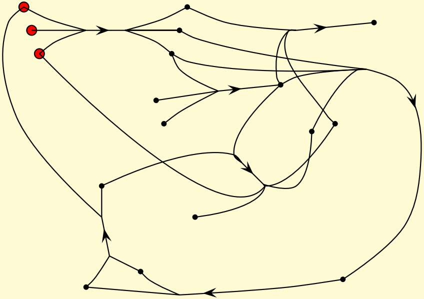
- $\mathcal{E}(H)$ is a set of ordered pairs $e = (t(e), h(e))$ of multisets $t(e), h(e)$ on $V(H)$, called *hyperarcs / reactions*
- $t(e)$ is the tail of e

Example



Definition

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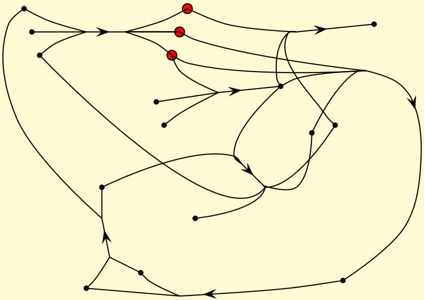
- $h(e)$ is the head of e

Example



Definition

A *homomorphism* from H_1 into H_2 is a mapping $\varphi : V(H_1) \to V(H_2)$ such that:

- $\varphi(E)$ is an arc in H_2 whenever E is an arc in H_1 with the property that $\varphi(t(E)) = t(\varphi(E))$ and $\varphi(h(E)) = h(\varphi(E))$

A mapping $\varphi : V(H_1) \to V(H_2)$ is a *weak homomorphism* if

- arcs are mapped either on arcs or on vertices

A bijective homomorphism φ whose inverse function is also a homomorphism is called an *isomorphism*.

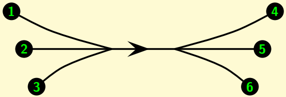
The bipartite digraph H_B of the dihypergraph H:

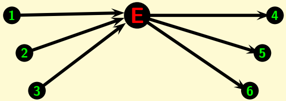
- $V(H_B) = V(H) \cup \mathcal{E}(H)$
- $(a, b) \in \mathcal{E}(H_B)$ if
  - $a \in \mathcal{E}(H)$ and $b \in h(a)$
  - $b \in \mathcal{E}(H)$ and $a \in t(b)$

Remark

$H_B \cong H$

Example





$E = (\{1, 2, 3\}, \{4, 5, 6\})$

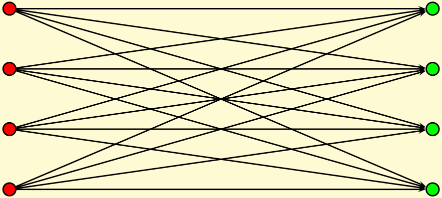
Species/Reaction Digraphs

Definition

The *complete bipartite digraph* $K(V_1, V_2)$:

- $e \in \mathcal{E}(K(V_1, V_2)) \Leftrightarrow h(e) \in V_1, t(e) \in V_2$
- $V(K(V_1, V_2)) = V_1 \cup V_2$

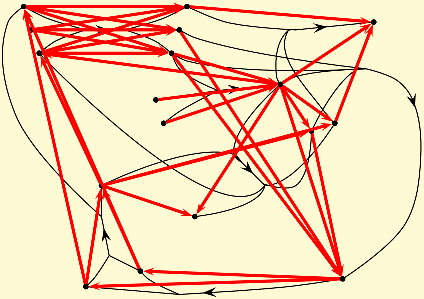
Example



Definition

The *species / substrate / underlying digraph* H_S of a dihypergraph H has the vertex set $V(H) = V(H_S)$ and $e = (v_i, v_j)$ is an element of $\mathcal{E}(H_S)$ iff there exists an $r \in \mathcal{E}(H)$ for which holds $v_i \in t(r), v_j \in h(r)$.

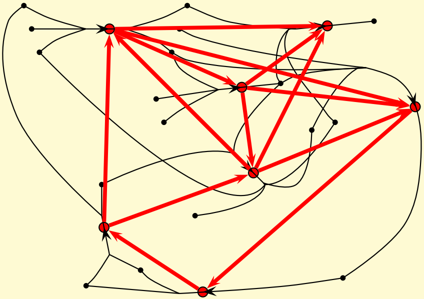
Example



Definition

The *reaction digraph* H_R of $H \in \mathcal{H}$ is the digraph with the vertex set $V(H_R) = \mathcal{E}(H)$. $e = (r_i, r_j)$ is an element of $\mathcal{E}(H_R)$ iff there are $r_i, r_j \in \mathcal{E}(H)$ with $h(r_i) \cap t(r_j) \neq \emptyset$.

Example



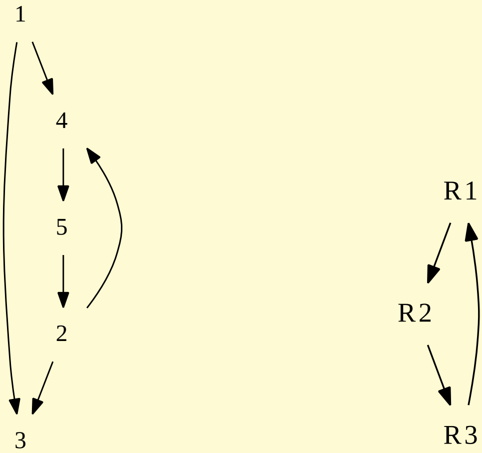
Definition

We assume S and R are digraphs.
$\ominus(H) = (H_S, H_R)$
$\oplus(S, R) = S \oplus R = \{H | \ominus(H) = (S, H_R), H_R \cong R\}$

Remark

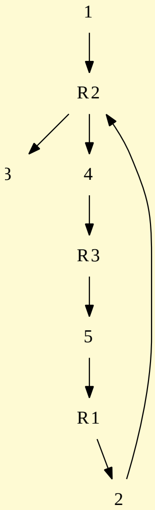
For every $(a, b) \in E(H_S)$ exists only one $e \in \mathcal{E}(H)$ with $a \in t(e)$ and $b \in h(e)$

Example



H_S and H_R

Example

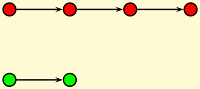


H

Remark

Given (S, R). If the minimal number of (maximal) complete bipartite disubgraph in S is greater than the number of vertices (reactions) in R then follows $S \oplus R = \emptyset$.

Example

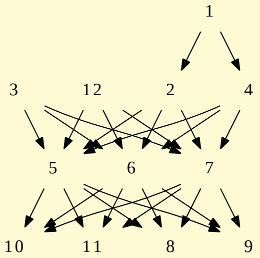


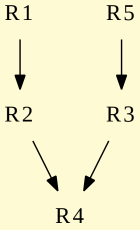
- number of complete bipartite digraphs is 3
- number of reactions is 2

Remark

Every dihypergraph determines a unique species and a unique reaction digraph but a species and reaction digraph together do not always determine a unique dihypergraph.

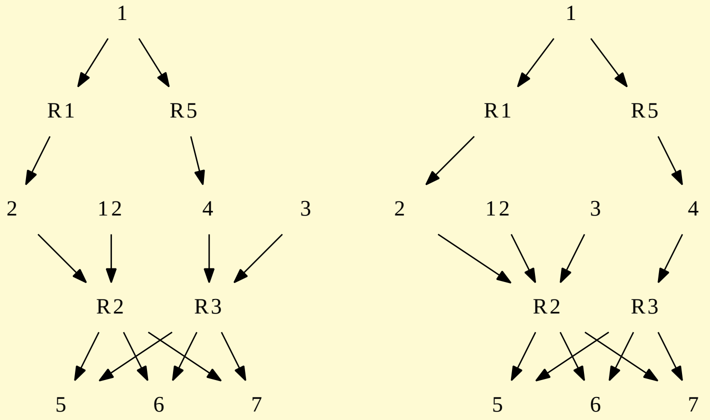
Example





S and R

Example

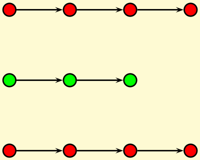


two elements of $S \oplus R$

Corollary

S, R are digraphs. If $R \cong LS \Rightarrow |S \oplus R| \geq 1$ and $S \in S \oplus R$.

Example



Definition

A *dipath* in a directed hypergraph H from a vertex u to vertex v is an alternating sequence of vertices and hyperarcs $x = (u = v_0, e_1, v_1, e_2, v_2, \ldots, e_k, v_k = v)$ such that for $1 \leq i, j \leq k$ holds:

- $v_{i-1} \in t(e_i)$ and $v_i \in h(e_i)$
- $e_i \neq e_j$ for $|i - j| < k$
- $v_i \neq v_j$ for $|i - j| < k$

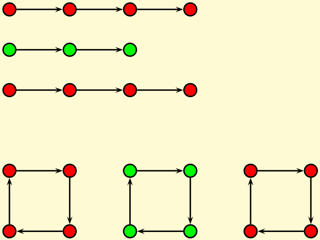
A dipath is a *dicycle* if also $u = v$.

Remark

Relations between cycles and paths:

- *Let* C_1, C_2 *be cycles in digraphs of same length,* $C_1 \oplus C_2 = C_1$
- *Let* P_1, P_2 *be paths in digraphs with* $|\mathcal{E}(P_1)| = n$ *and* $|\mathcal{E}(P_2)| = n - 1$, $P_1 \oplus P_2 = P_1$

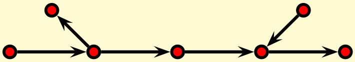
Example

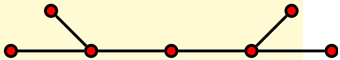


Definition

U is the mapping $U : \mathcal{D} \to \mathcal{U}$ which is given by $U(V(G), \mathcal{E}(G)) = (V(G), E(G))$ such that every arc $(a, b) \in \mathcal{E}(G)$ will be mapped to $\{a, b\} \in E(G)$.

Example





G and $U(G)$

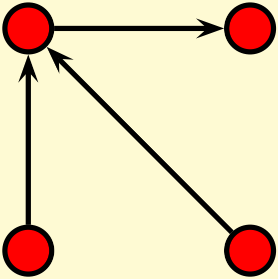
Remark

$H \in \mathcal{H}$. If there is no isolated node in $U(H_R)$ then every arc in H is contained in a dipath of length 2.

Corollary

$H \in \mathcal{H}$. If $U(H_S)$ is connected and $U(H_R)$ is the union of at least two vertex-disjoint cycles, then exists no dicycle in H.

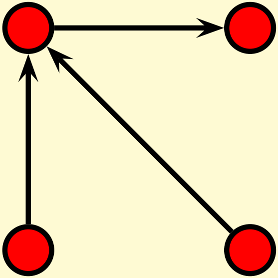
Example



Corollary

H is a dihypergraph. If $U(H_S)$ is connected and $U(H_R)$ is the vertex-disjoint union of cycles and cycle-free connected components, then follows H is dicycle-free.

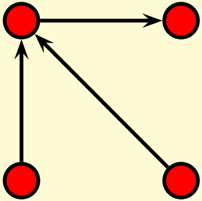
Example



Corollary

Let H be a hypergraph such that $U(H_S)$ is connected and $U(H_R)$ is the union of k vertex-disjoint graphs $\{G_1, \ldots, G_k\}$. There is no dicycle in H with arc set $\mathcal{E}(G_i)$, $1 \leq i \leq k$.

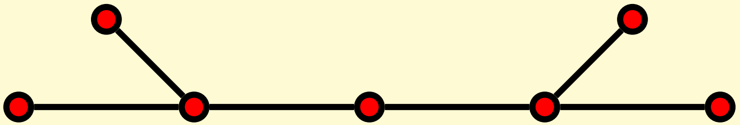
Example



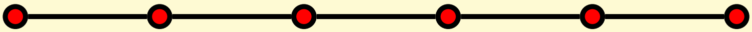
Remark

n-cycles can occur in a species graph S such that there are no n-cycles in the reaction graph R and $S \oplus R \neq \emptyset$.

Example

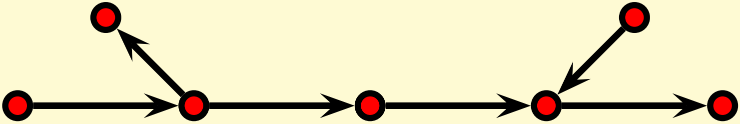


S_1



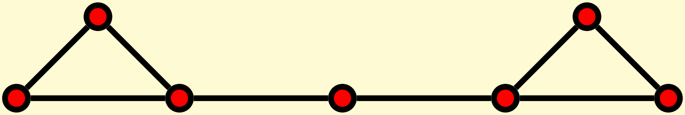
R_1

Example



$\{H\} = S_1 \oplus R_1$

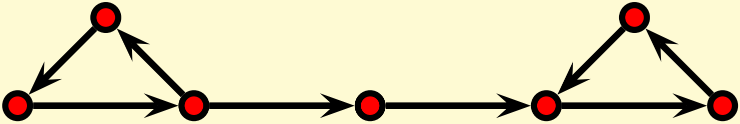
Example



S_2

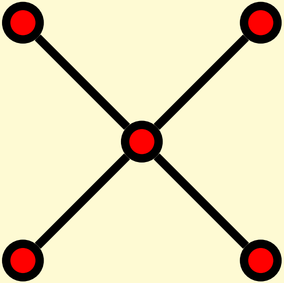
R_2

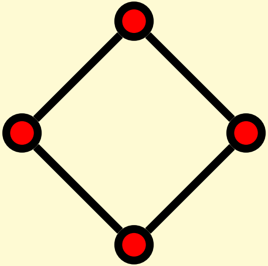
Example



$\{H\} = S_2 \oplus R_2$

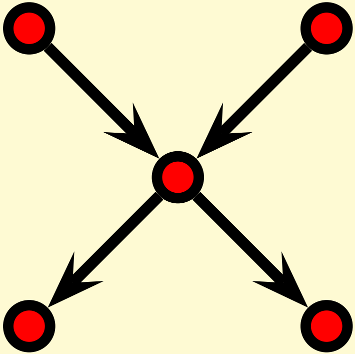
Example





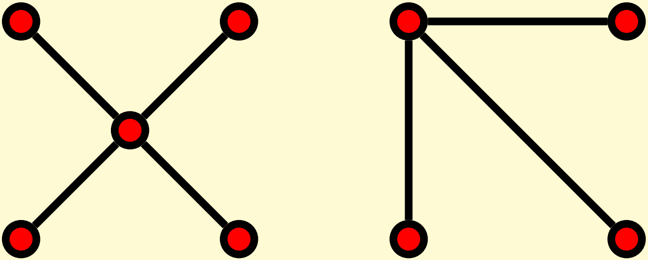
S_3 and R_3

Example

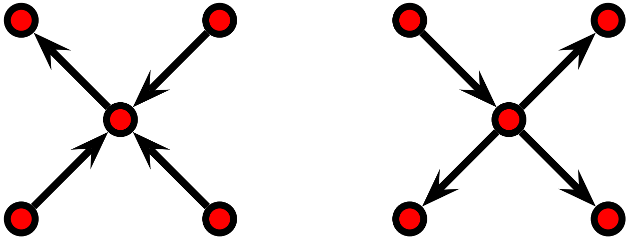


$\{H\} = S_3 \oplus R_3$

Example

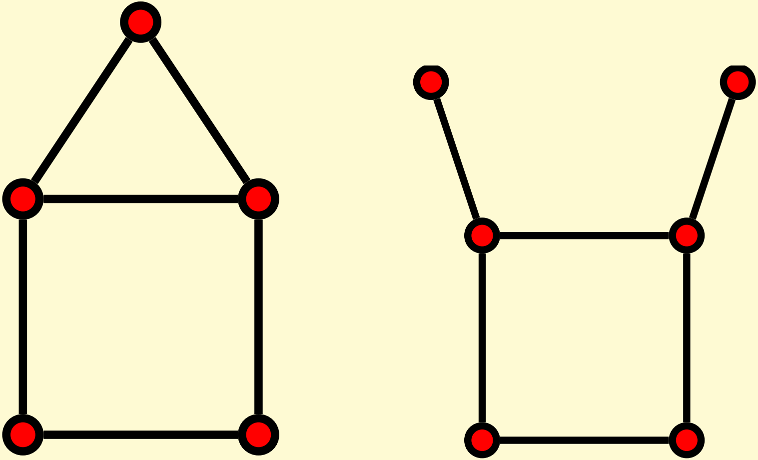


S_4 and R_4



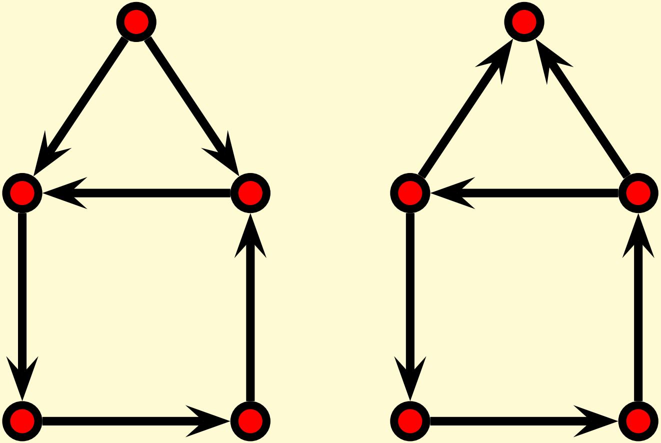
$\{H_1, H_2\} = S_4 \oplus R_4$

Example



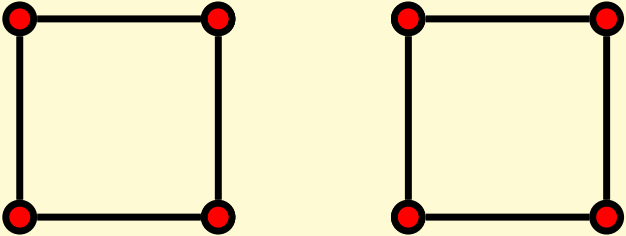
S_5 and R_5

Example



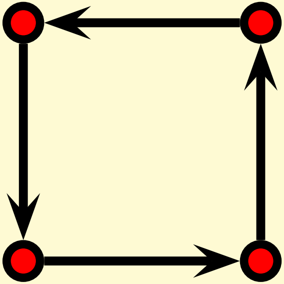
$\{H_1, H_2\} = S_5 \oplus R_5$

Example



S_6 and R_6

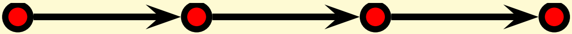
Example



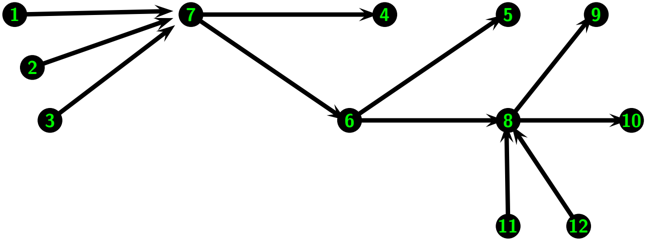
$\{H\} = S_6 \oplus R_6$

Example

S_7 and R_7



$\{H\} = S_7 \oplus R_7$


1
2
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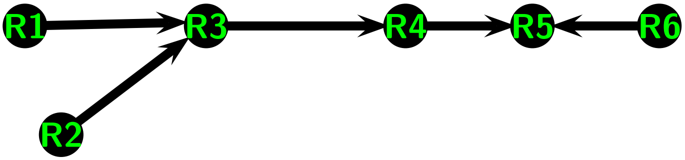
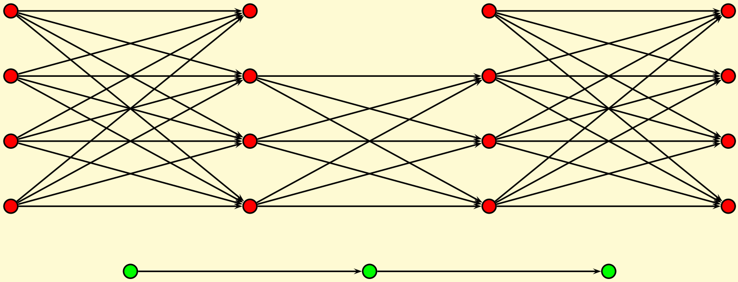
12

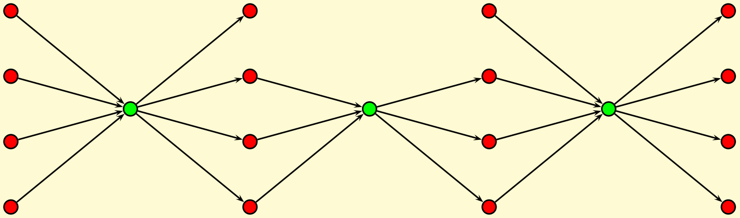

R1
R2
R3
R4
R5
R6

Example

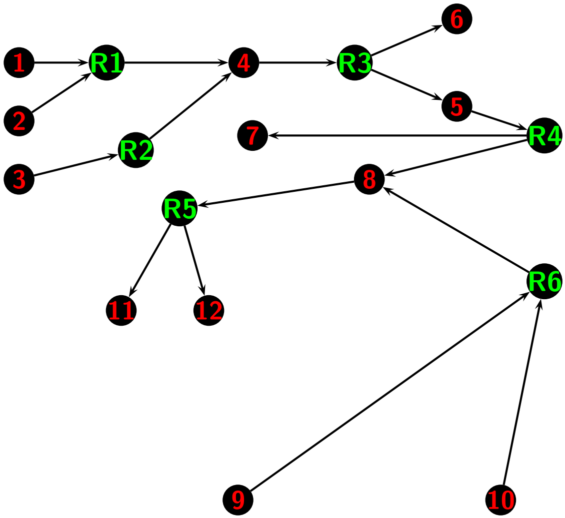


S and R

Example



$\{H\} = S \oplus R$


6
1
R1
4
R3
2
5
R4
7
R2
3
8
R5
R6
11
12
9
10

Thanks for your attention!!!

Thanks to Jürgen, Peter F., Pierre-Yves, Lydia, Christoph, Marc, Alex, Nick, Bruno, Daniel, Steve, Börni, Abdullah,.....!