Graph Theory

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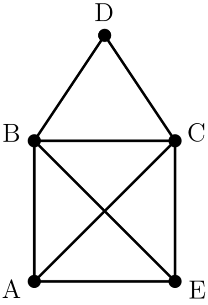
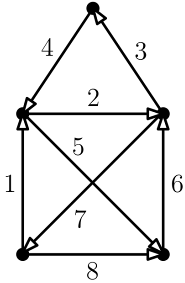
1 Introduction

A formal definition will follow. In general:

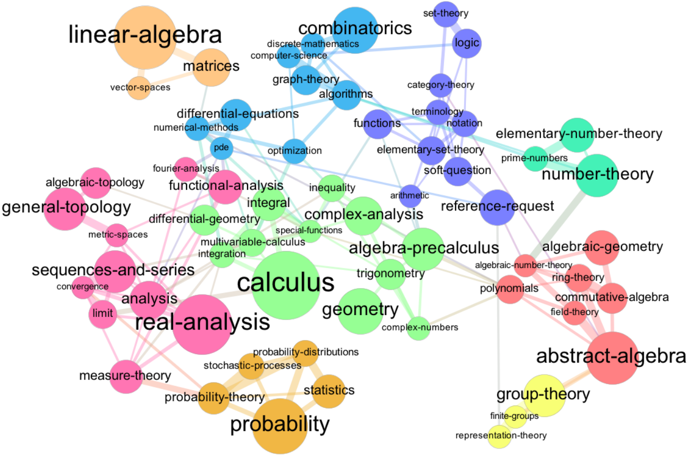
A **Graph** is a network with **nodes** and **edges**.





Important:

Graph theory is a field in **discrete mathematics**. In physics, mathematics, biology, life sciences and further areas, the concept of a **graph** is often denoted as **network**. We will hence use both terms synonymously.



Source: https://math.meta.stackexchange.com/questions/6479/a-graph-map-of-math-se


Bahnen in Köln
Rail Services Cologne
2022
Stadtbahnlinie
tram / light railway
S-Bahn
rail rapid transit
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Merkenich
Endhaltestelle
terminus
Niehl Nord
alternative Endhaltestelle
alternative terminus
kein barrierefreier Zugang an mind. einer Linie
no barrier-free access at least one line
P+R-Platz
park and ride
Tarifgrenze
fare zone boundary
Stand: 2021-12
0180 6 50 40 30
www.kvb.koeln


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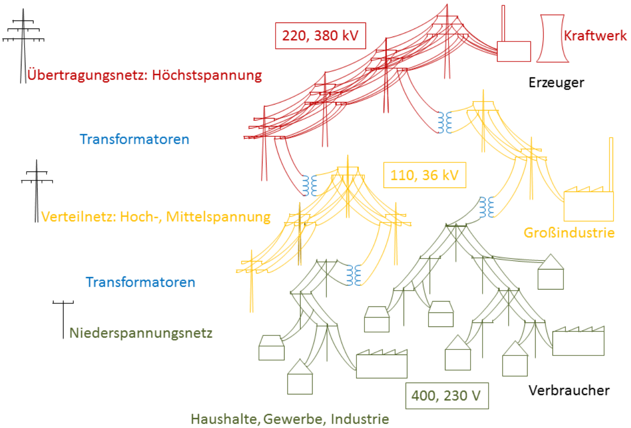
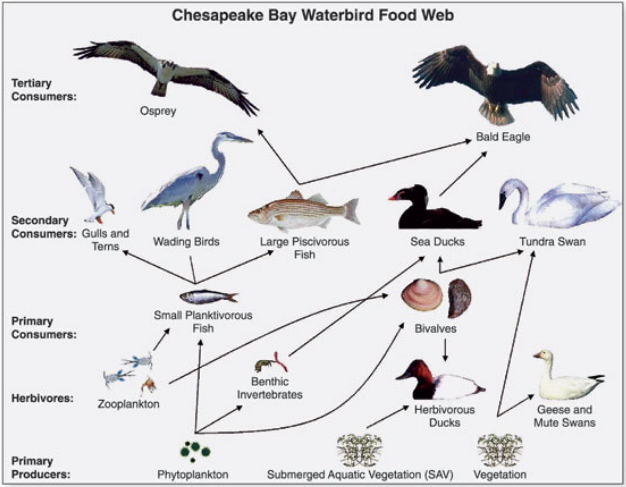
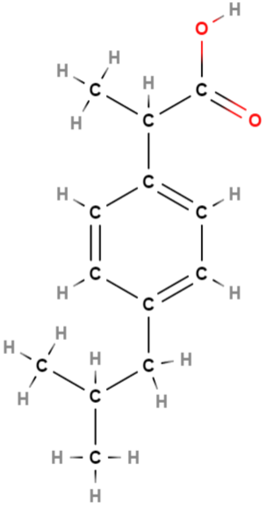


Source: http://www.regenerative-zukunft.de/joomla/stromnetzausbau


Chesapeake Bay Waterbird Food Web
Tertiary Consumers:
Osprey
Bald Eagle
Secondary Consumers:
Gulls and Terns
Wading Birds
Large Piscivorous Fish
Sea Ducks
Tundra Swan
Primary Consumers:
Small Planktivorous Fish
Bivalves
Herbivores:
Zooplankton
Benthic Invertebrates
Herbivorous Ducks
Geese and Mute Swans
Primary Producers:
Phytoplankton
Submerged Aquatic Vegetation (SAV)
Vegetation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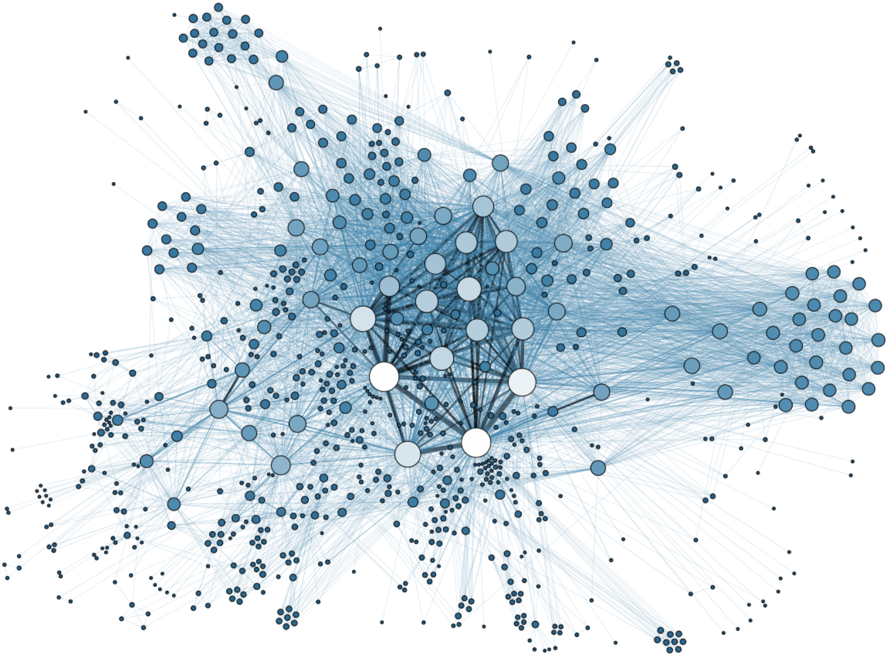

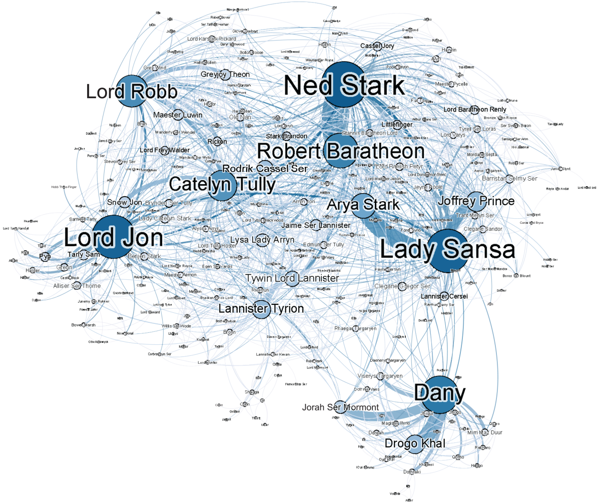

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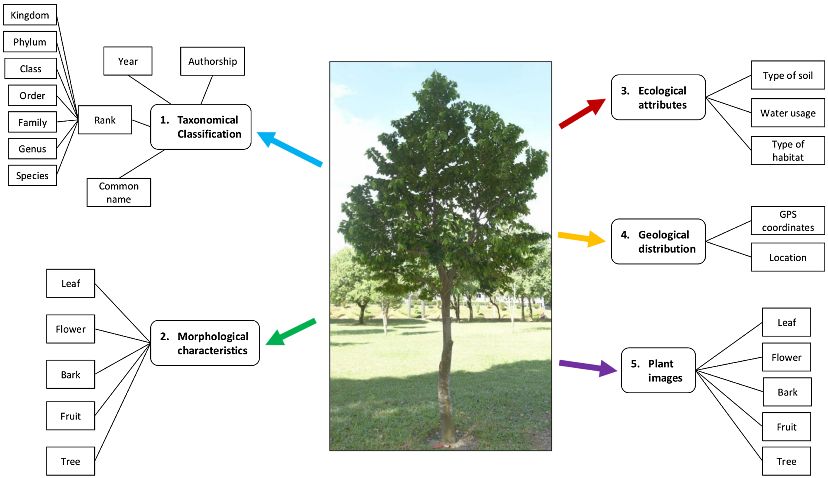
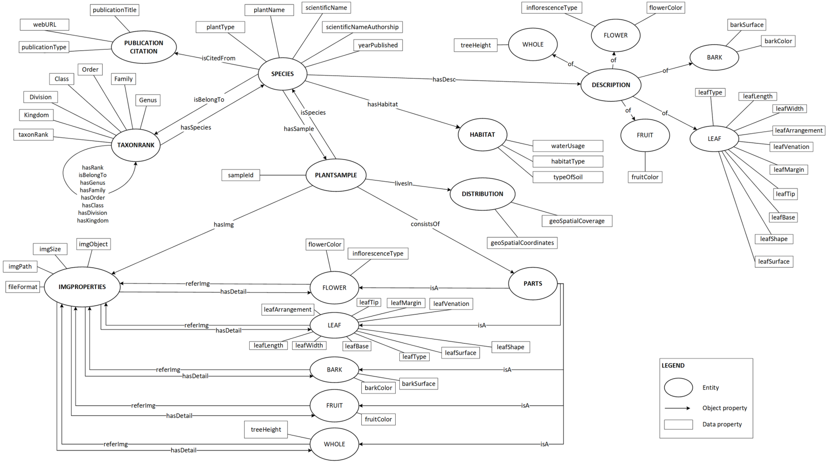


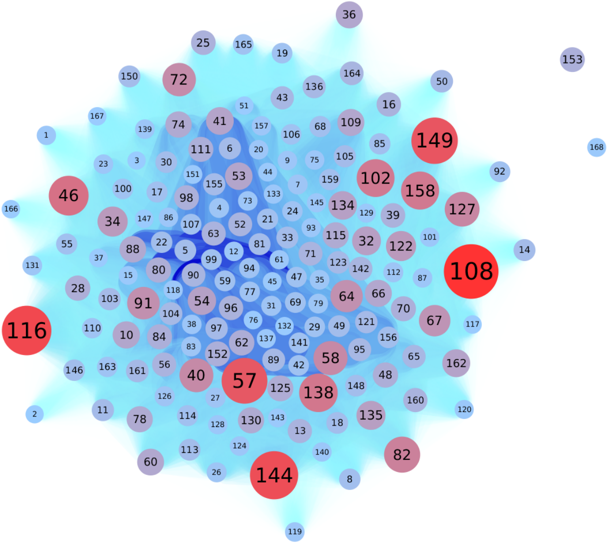
„Plant data description."

Source: https://doi.org/10.7717/peerj.5579/fig-2 schema.png



„The plant data description translated into ontology in a graph format.“

Source: https://doi.org/10.7717/peerj.5579/fig-4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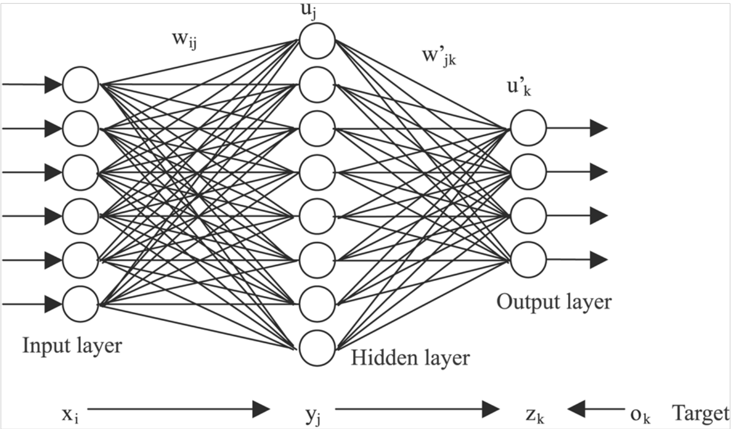
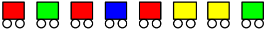
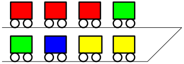
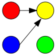
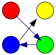


Source: https://math.stackexchange.com/tags/neural-networks/info

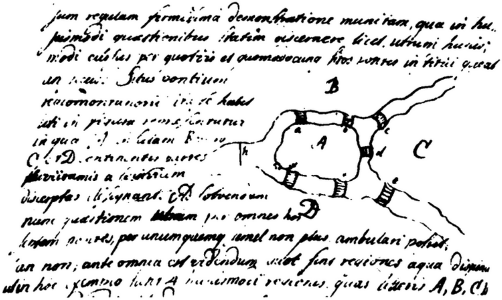
σ 



$D(S)$  $D^*(S)$ 

- Graphs are an universal concept with applications in countless scientific domains.
- But it is in any case an interdisciplinary field:
    - Graph theory is a mathematical field related to optimization, combinatorics and discrete mathematics.
    - Algorithmic graph theory can be considered as part of computer science related to efficient algorithms.
    - Graphs are also related to artificial intelligence, in particular neuronal networks and machine learning. This is either related to statistics or computer science.
    - Knowledge Graphs are a concept which is also used within Data Science and Digital Humanities.
- We will now continue with formal definitions and foundations.

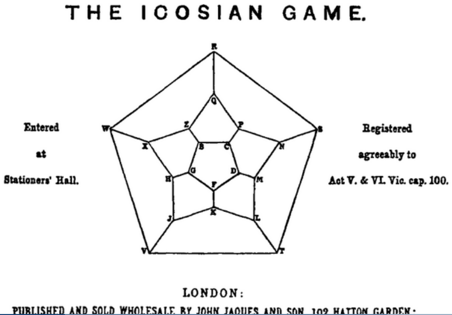
- I will present some (actually: only a few) notes on the history of Graph Theory.
- "Officially" Graph Theory began with Euler and the *Königsberg bridges problem*:
- Is it possible to find a route crossing each of the seven bridges of Königsberg once and once only?



- R. J. Wilson 1999, 503:

  The origins of graph theory are humble, even frivolous. Whereas many branches of mathematics were motivated by fundamental problems of calculation, motion, and measurement, the problems which led to the development of graph theory were often little more than puzzles, designed to test the ingenuity rather than to stimulate the imagination. But despite the apparent triviality of such puzzles, they captured the interest of mathematicians, with the result that graph theory has become a subject rich in theoretical results of a surprising variety and depth.

- E.g. Hamilton graphs:

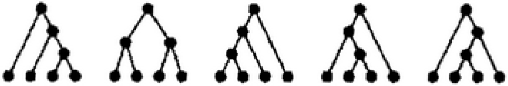


- Robin Wilson / John J. Watkins: Combinatorics: ancient & modern 2013:

  Early work on the generation of combinatorial patterns began as civilization itself was taking shape. The story is quite fascinating, [...] it spans many cultures in many parts of the world, with ties to poetry, music ans religion.

- But:

  The trees most dearly beloved by computer scientists – binary trees, or the equivalent ordered forests or nested parentheses – are strangely absent from the literature.



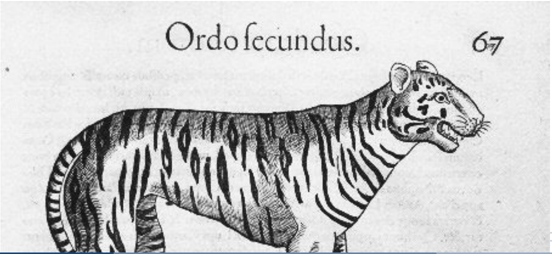
- Sebastian Gießmann: Graphen können alles: Visuelle Modellierung und Netzwerktheorie vor 1900 (2008):

  > *Formally, graph theory as network theory would have been widely applicable to phenomena in nature, technology and society much earlier. That this happens only in the 20th century and then, quite rapidly, raises further questions. (translated from German)*

- But: Is ‘network thinking’ related to modern times?

- Aristotle (384–322 BC):

  Very extensive genera of animals, into which other subdivisions fall, are the following: one, of birds; one, of fishes; and another, of cetaceans. Now all these creatures are blooded.
  There is another genus of the hard-shell kind, which is called oyster; another of the soft-shell kind, not as yet designated by a single term, such as the spiny crawfish and the various kinds of crabs and lobsters; and another of molluscs, as the two kinds of calamary and the cuttle-fish; that of insects is different. All these latter creatures are bloodless, and such of them as have feet have a goodly number of them; and of the insects some have wings as well as feet.
  (Historia animalium I.6.)



Early in this century the Hungarian Emil Torday lived for some time among the Shongo people in the Congo area. One day he went up to a circle of small children playing with sand. [...] The task was to draw each of the figures in the sand without lifting the finger or retracing any line segment. (Zaslavsky, Africa Counts (1999):105ff)

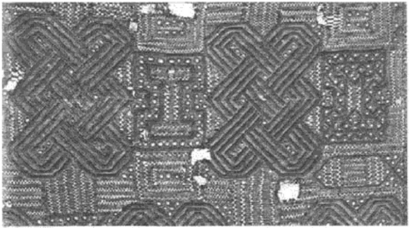
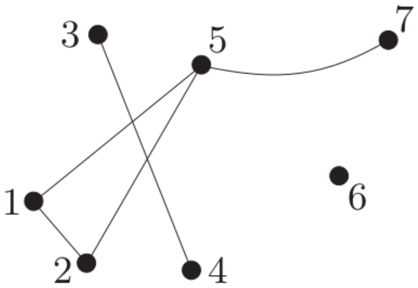


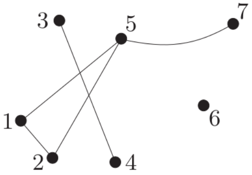
Figure 10-6 Kuba (Shongo) embroidered raffia cloth, Zaire (Congo). The interlacing mbolo *pattern is similar to those drawn in the sand by Kuba children. This cloth dates back to the eighteenth century. British Museum.*

Definition 1.1

We call $G = (V, E)$ a graph where V denotes the set of vertices (or nodes) and E denotes the set of edges.



The Graph on $V = \{1, ..., 7\}$ with edge set
$E = \{\{1, 2\}, \{1, 5\}, \{2, 5\}, \{3, 4\}, \{5, 7\}\}$.



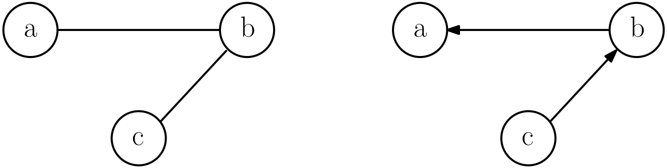
- A graph with vertex set V is said to be a graph on V.
- The vertex set of a graph G is referred to as $V(G)$, its edge set as $E(G)$.
- In general the number of vertices is called the *order* of G and denoted by $|V| = n$ (rarely: $|G|$).
- We usually denote $|E| = m$.
- Graphs may be *finite, infinite* or *countable*.
- Two nodes $u, v \in V$ are *adjacent* or *neighbors*, if an edge $\{u, v\} \in E$ exists.
- A vertex v is *incident* with an edge e if $v \in e$; then e is an edge at v.

- A graph G is called *directed* (or *digraph*) if edges have a direction.

  In this case, $(u, v) \neq (v, u)$.
- For the directed edge (u, v), u is called the *tail* and v the *head*.
- A graph is *undirected* if edges have no direction.

  This means, in an undirected graph $(u, v) \in E \Leftrightarrow (v, u) \in E$.

  Whenever we draw a directed graph, the edges have a direction which is displayed by an arrow.

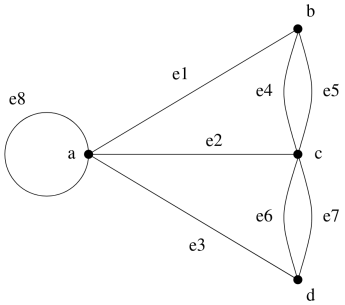


Definition 1.2

An edge $e \in E$ is called *loop* if and only if e is incident with only one node.

Definition 1.3

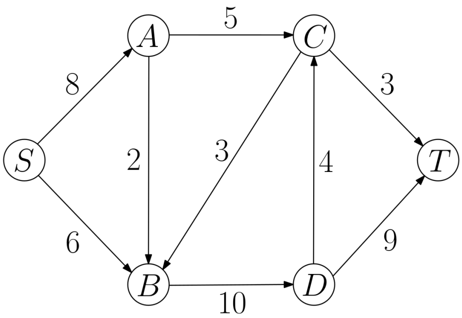
Two edges $e_1, e_2 \in E$ are called *parallel* if and only if they are incident to the same nodes.



$$V = \{a, b, c, d\}, \quad E = \{e_1, e_2, ..., e_8\}$$

Definition 1.4

A *weighted graph* is a graph in which each edge is given a numerical weight. The *weight* of the edge set E is defined by a weight function $w : E \to \mathbb{R}$.



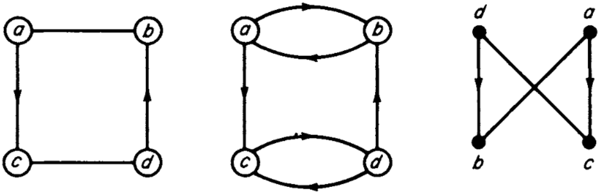
The weight of an edge can e.g. represent a capacity, cost or distance. In the different areas of application we will also adjust the names, for example length or dist(ance) instead of weight and limit them to integers, or non-negative numbers.

Definition 1.5

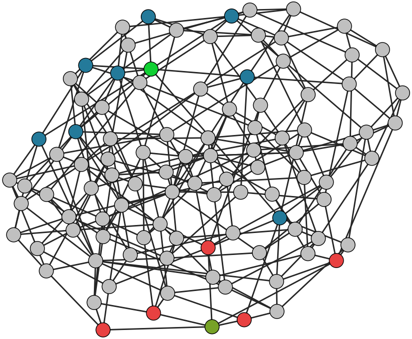
A simple graph, is an unweighted, undirected graph containing no graph loops or multiple edges.

- A simple graph may be either connected or disconnected.
- Unless stated otherwise, the unqualified term ‘graph’ usually refers to a simple graph.
- A simple graph with multiple edges is sometimes called a multigraph.

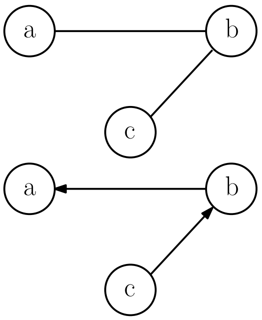
It is often convenient to draw a ‘picture’ of the graph. This may be done in many ways.



Our figures are meant simply as a tool to help understand the underlying mathematical structure or as an aid in constructing a mathematical model for some application (See: Golumbic 3-4).



- The *neighborhood* $N(v)$ of a vertex $v \in V$ is the set of all nodes connected to v, which means $N(v) = \{u \in V | \{u, v\} \in E\}$.
- The neighborhood in which the vertex $v \in V$ itself is included is called the *closed neighborhood* $N[v] = N(v) \cup \{v\}$.



Example 1.6

The neighborhood of b consists of the nodes a and c, for short $N(b) = \{a, c\}$. If we consider the directed graph, $N^-(b) = \{c\}$ and $N^+(b) = \{a\}$.

- The *degree* of a vertex $v \in V$ is the number of nodes adjacent to v and is denoted by $d(v)$, $deg(v)$ or $\delta(v)$.

  Thus, if G is an undirected graph, $deg(v) = |N(v)|$.

  If G is a directed graph, we differ between indegree and outdegree.

  For every node $v \in V$ the *indegree* $deg^-(v) = |N^-(v)|$ is the number of incoming edges (x, v) to v,

  with $N^-(v) = \{x \in V, (x, v) \in E\}$.

  Analogously, $N^+(v) = \{x \in V, (v, x) \in E\}$ is the set of all outgoing edges

  and thus the *outdegree* is $deg^+(v) = |N^+(v)|$.
- A graph G is called *complete graph* if for all nodes $u, v \in V$ the edge $\{u, v\}$ exists in E.

- A vertex of degree 0 is *isolated*.
- Minimum degree: $\delta(G) = \min\{d(v) | v \in V\}$
- Maximum degree: $\Delta(G) = \max\{d(v) | v \in V\}$
- If all the vertices of G have the same degree k, then G is called *k-regular*.
- Average degree of G:

$$d(G) = \frac{1}{|V|} \sum_{v \in V} d(v)$$

Lemma 1.7 (Euler's Handshaking Lemma)

For any graph:

$$\sum_{v \in V} d(v) = 2|E|$$

Lemma 1.8

Every graph has an even number of vertices of odd valency.

Proof.

Let $V_e := \{v \in V | deg(v) \ even\}$ and
$V_o := \{v \in V | deg(v) \ odd\}$.
Handshaking Lemma:

$$\begin{aligned} 2|E| &= \sum_{v \in V} d(v) \\ &= \sum_{v \in V_e} d(v) + \sum_{v \in V_o} d(v) \end{aligned}$$

since $V = V_e + V_o$
$\Rightarrow \sum_{v \in V_o} d(v)$ is even (since V_e and $2|E|$ even)
$\Rightarrow |V_o|$ even. $\square$

Let $G = (V, E)$ and $G' = (V', E')$ be two graphs.

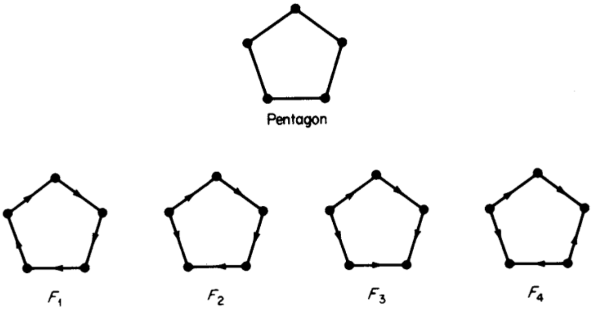
Definition 1.9

A map $\varphi : V \to V'$ is a *homomorphism* from G to G' if it preserves the adjacency of vertices, that is, if $\{\varphi(x), \varphi(y)\} \in E'$ whenever $\{x, y\} \in E$.

Definition 1.10

If φ is bijective and its inverse φ^{-1} is also a homomorphism (so that $xy \in E \Leftrightarrow \varphi(x)\varphi(y) \in E' \;\; \forall\, x, y \in V$), we call φ an isomorphism, say that G and G' are *isomorphic*, and write $G \simeq G'$. An isomorphism from G to itself is an *automorphism* of G.

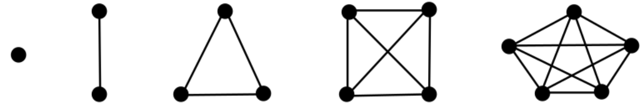
We do not normally distinguish between isomorphic graphs. Thus, we usually write $G = G'$ rather than $G \simeq G'$, speak of the complete graph on 17 vertices, and so on.



The four nonisomorphic orientations of the pentagon.

Definition 1.11

A graph is *complete* if every pair of distinct vertices is adjacent.
The complete graph on n vertices is usually denoted by K_n.



K_1 K_2 K_3 K_4 K_5

Definition 1.12

A class of graphs that is closed under isomorphism is called a *graph property*.

Example 1.13

- containing a triangle

Definition 1.14

A map taking graphs as arguments is called a *graph invariant* if it assigns equal values to isomorphic graphs.

Example 1.15

The number of vertices and the number of edges of a graph are two simple graph invariants; the greatest number of pairwise adjacent vertices is another.

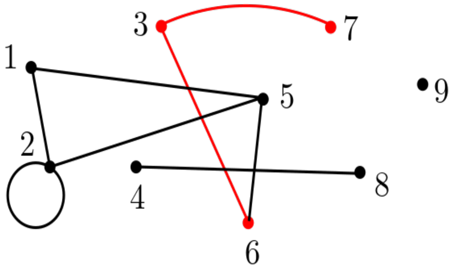
- $G \cup G' = (V \cup V', E \cup E')$
- $G \cap G' = (V \cap V', E \cap E')$

Definition 1.16

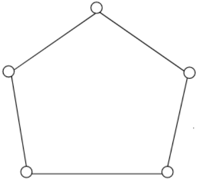
If $G \cap G' = \emptyset$ then G and G' are called *disjoint*.

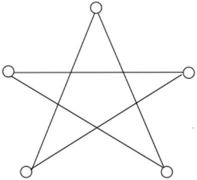
Definition 1.17

If $V' \subseteq V$ and $E' \subseteq E$ then G' is a *subgraph* of G, denoted by $G' \subseteq G$, and G a *supergraph* of G'.



Red: $H = \left(\tilde{V}, \tilde{E}\right) \subseteq G$, with $V = \{3, 6, 7\}$ and $E = \{(3,6), (3,7)\}$





- Let $G = (V, E)$ be a simple graph.
- $\overline{G}$ is called the *complement* of G with $V(G) = V(\overline{G})$ and

$$e \in E(\overline{G}) \Leftrightarrow e \notin E(G)$$

- We denote $(V, E \setminus F)$ with $G - F$ and
- $G - e$ instead of $G - \{e\}$.
- Let $F \subseteq V \times V$, then we denote $(V, E \cup F)$ with $G + F$ and
- $G + e$ instead of $G + \{e\}$.

- If $G' \subseteq G$ and G' contains all the edges $xy \in E$ with $x, y \in V'$, then G' is an induced subgraph of G; we say that V' induces or spans G' in G, and write

$$G' = G[V']$$

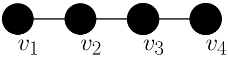
- Thus if $U \subseteq V$ is any set of vertices, then $G[U]$ denotes the graph on U whose edges are precisely the edges of G with both ends in U.
- If H is a subgraph of G, not necessarily induced, we abbreviate $G[V(H)]$ to $G[H]$.
- Finally, $G' \subseteq G$ is a *spanning* subgraph of G if V' spans all of G, i.e. if $V' = V$.

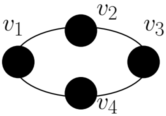
Definition 1.18

A *path* p is a set of pairwise adjacent vertices $v_1, ..., v_n$, for example written as

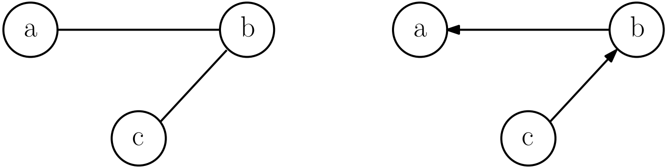
$$p = [v_1, ..., v_n],$$

where $(v_i, v_{i+1}) \in E$ for $i \in \{1, \dots, n-1\}$.





- The length $|p|$ of p is the total number of edges, hence $|p| = n - 1$.
- The path p links the starting vertex v_1 and the ending vertex v_n.
- In a path, $v_i \neq v_j$ for all $i, j \in \{1, ...n\}$.
- If $v_1 = v_n$, we no longer speak about paths. In this case, we consider *circles*.



Example 1.19

Example paths are

$$p = [a, b, c]$$

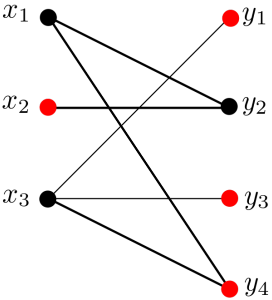
$$p' = [c, b, a]$$

If we consider the directed graph on the right side, p is no longer a path of the graph, since the edges are directed.

- A sequence of vertices $[v_0, v_1, ..., v_l, v_0]$ is called a *cycle* of length $l + 1$ if $(v_{i-1}, v_i) \in E$ for $i \in \{1, ..., l\}$ and $(v_l, v_0) \in E$.
- A cycle $[v_0, v_1, ..., v_l, v_0]$ is a *simple cycle* if $v_i \neq v_j$ for $i \neq j$.
- A simple cycle $[v_0, v_1, ..., v_l, v_0]$ is *chordless* if $(v_i, v_j) \notin E$ for i and j differing by more than $1 \mod l + 1$.

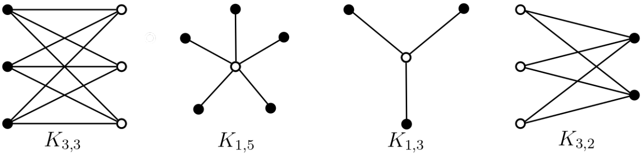
- A subset $A \subseteq V$ of r vertices is an *r-clique* (or: *complete set*) if it induces a complete subgraph, i.e. if $G_A \simeq K_r$.
- A single vertex is a 1-clique.
- A clique A is maximal if there is no clique of G which properly contains A in a subset.
- A clique is maximum if there is no clique of G of larger cardinality.
- $\omega(G)$ is the number of vertices in a maximum clique of G; it is called the *clique number* of G.
- $k(G)$ is the size of a smallest possible clique cover of G; it is called the *clique cover number* of G.

- A *stable* set (or: *independent set*) is a subset X of vertices no two of which are adjacent.
- $\alpha(G)$ is the number of vertices in a stable set of maximum cardinality; it is called the *stability number* of G.

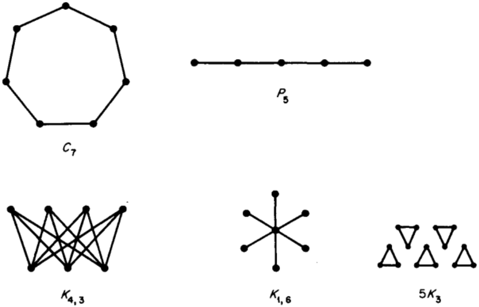


Red: Maximum stable set $X = \{x_2, y_1, y_3, y_4\} \subseteq V$, $\alpha(G) = 4$

- An undirected graph $G = (K, E)$ is bipartite if its vertices can be partitioned into two disjoint stable sets $V = S_1 + S_2$, i.e., every edge has one endpoint in S_1 and the other in S_2. Equivalently, G is bipartite if and only if it is 2-colorable. It is customary to use the notation $G = (S_1, S_2, E)$, which emphasizes the partition.
- A bipartite graph $G = (S_1, S_2, E)$ is complete if for every $x \in S_1$ and $y \in S_2$ we have $(x, y) \in E$, i.e., every possible edge that could exist does exist.



- K_n the complete graph on n vertices or n-clique.
- C_n the chordless cycle on n vertices or n-cycle.
- P_n the chordless path graph on n vertices or n-path.
- $K_{m,n}$ the complete bipartite graph on $m + n$ vertices partitioned into an m-stable set and an n-stable set.
- $K_{1,n}$ the star graph on $n + 1$ vertices.
- mK_n m disjoint copies of K_n.

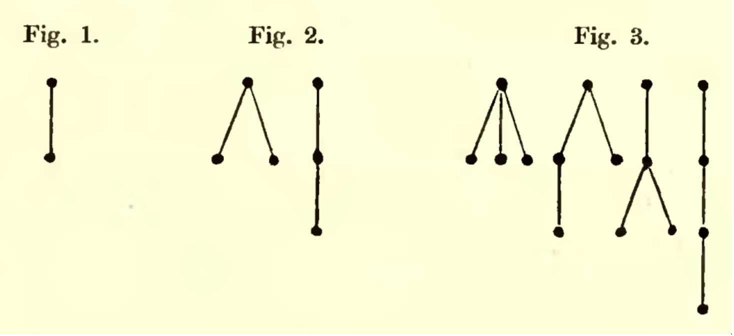


Definition 1.20

A graph G is called *connected* if it is non-empty and any two of its vertices are linked by a path in G.

- If $U \subseteq V(G)$ and $G[U]$ is connected, we also call U itself connected (in G).
- Instead of 'not connected' we usually say 'disconnected'.

- An *acyclic* graph, one not containing any cycles, is called a *forest*.
- A connected forest is called a *tree*.
- The vertices of degree 1 in a tree are its *leaves*, the others are its inner vertices.



Theorem 1.21

The following assertions are equivalent for a graph T:

1. *T is a tree;*
2. *Any two vertices of T are linked by a unique path in T;*
3. *T is minimally connected, i.e. T is connected but $T - e$ is disconnected for every edge $e \in T$;*
4. *T is maximally acyclic, i.e. T contains no cycle but $T + xy$ does, for any two non-adjacent vertices $x, y \in T$.*

Proof.

(1)$\Rightarrow$(2):
Let T be a tree.

- Suppose, for the purpose of contradiction, that there are distinct vertices x and y in T that are not connected by a unique path in T.
- If they are not connected at all, then T is disconnected, which is a contradiction with the fact that T is a tree.
- Assume, then, that there are distinct xy-paths P_1 and P_2.
- Denote by z the vertex of least distance from x such that $z \neq x$ and z belongs to both P_1 and P_2.
- Observe that such a vertex is guaranteed to exist, as $y \neq x$ and y belongs to both P_1 and P_2.
- Now, xP_1zP_2x is a cycle in T, which is a contradiction with the fact that T is a tree.
- Therefore, any two vertices in T are linked by a unique path in T.

□

Lemma 1.22

The vertices of a tree can always be enumerated, say as $v_1, \ldots, v_n$, so that every v_i with $i \geq 2$ has a unique neighbour in $\{v_1, \ldots, v_{n-1}\}$.

Lemma 1.23

A connected graph with n vertices is a tree if and only if it has $n-1$ edges.

Proof.

Induction on i shows that the subgraph spanned by the first i vertices in lemma 1.22 has $i-1$ edges; for $i = n$ this proves the forward implication.
Conversely, let G be any connected graph with n vertices and $n-1$ edges. Let G' be a spanning tree in G. Since G' has $n-1$ edges by the first implication, it follows that $G = G'$. □