

Martin Loebel

# Discrete Mathematics in Statistical Physics

Introductory Lectures





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Introductory Lectures



Dr. Martin Loebel  
Charles University  
Department of Applied Mathematics  
Institut of Theoretical Computer Science  
Malostranske 25  
CZ-118 00 Praha  
Tschechische Republik  
E-Mail: [loebel@kam.mff.cuni.cz](mailto:loebel@kam.mff.cuni.cz)

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dedicated to Zbyněk and Jaroslava, my parents

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## Preface

The purpose of these lecture notes is to briefly describe some of the basic concepts interlacing discrete mathematics, statistical physics and knot theory. I tried to emphasize a 'combinatorial common sense' as the main method. No attempt of completeness was made. The book should be accessible to the students of both mathematics and physics. I profited from previous books and expositions on discrete mathematics, statistical physics, knot theory and others, namely [B1], [BRJ], [BB], [J1], [KG], [LL], [MN], [MJ], [MT], [S0], [S3], [SM], [WFY], [WD], [KSV]. Most of the material contained in the book is introductory and appears without a reference to the original source. This book has been an idea of my editor Martin Aigner. I would like to thank to him for his support and help. Many other colleagues helped me with the book. Mihyun Kang, Jirka Matoušek, Iain Moffatt, Jarik Nešetřil, Dominic Welsh and Christian Krattenthaler read earlier versions, and without their extensive comments the book would probably not exist. I had enlightening discussions on several topics discussed in the book, in particular with Martin Klazar, Roman Kotecký, Ondřej Pangrác, Gregor Masbaum, Xavier Viennot and Uli Wagner. Marcos Kiwi saved the whole project by gently teaching me how to draw pictures and Winfried Hochstaettler drew one; I am sure you will be able to detect it. Large part of the book was written during my visit, in the whole year 2006, at the School of Mathematics and the Centro Modelamiento Matematico, Universidad de Chile. I want to thank my colleagues there for wonderful hospitality, and gratefully acknowledge the support of CONICYT via project Anillo en Redes, ACT-08. But of course, the seminal ingredient in the process of making the book was the creative environment of my home department of applied mathematics and the institute of theoretical computer science at the Charles University, Prague. Some theorems and observations in the book appear without a proof. Usually a pointer is given to a book (preferentially) or to a paper where a proof can be found. If no pointer is given, then I believe (possibly mistakenly) that it should be possible to prove the statement in an elementary and not very complicated way. The reader is encouraged to write down such proofs as exercises. The first five chapters concentrate on the introductory discrete mathematics. Chapters six and seven are devoted to the partition functions, and chapter eight is an introduction to the theory of knots. The last chapter describes two combinatorial technics which solve the 2D Ising and dimer problems.

Prague, September 2009  
Martin Loeb1

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# Chapter 1

## Basic concepts

In this introductory chapter we first present some very basic mathematical formalism. Then we introduce algorithms and complexity. The chapter ends with basic tools of discrete calculations.

### 1.1 Sets, functions, structures

We will use symbols  $\mathbb{N}, \mathbb{Z}, \mathbb{P}, \mathbb{Q}, \mathbb{R}$ , and  $\mathbb{C}$  to denote the sets of the natural, integer, positive integer, rational, real, and complex numbers. If not specified otherwise then  $i, j, k, m, n$  are non-negative integers. We sometimes denote by  $[n]$  the set  $\{1, \dots, n\}$ . We denote by  $|X|$  the cardinality of a set  $X$ . A function  $f$  from a set  $X$  to a set  $Y$  is called *one-to-one* or *injective* if  $x, y \in X, x \neq y$  implies  $f(x) \neq f(y)$ , it is *surjective* or *onto* if for each  $y \in Y$  there is  $x \in X$  such that  $f(x) = y$ , and it is a *bijection* if it is both one-to-one and onto. If  $X, Y$  are finite then a bijection is also called a *permutation*. Let  $|X| = n$  and  $|Y| = m$ . There are  $n! = n(n-1)(n-2) \cdots 1$  permutations of  $X$ ;  $n!$  is the *factorial function*. The number of all functions from  $X$  to  $Y$  is  $m^n$  and the number of one-to-one functions from  $X$  to  $Y$  is  $m(m-1) \cdots (m-n+1)$ . The number of surjective functions does not have such a nice formula, it may be written with the help of the principle of inclusion and exclusion as

$$\sum_{i=0}^m (-1)^i \binom{m}{i} (m-i)^n. \quad (1.1)$$

The *Kronecker delta function* is defined by  $\delta(x, y) = 1$  if  $x = y$ , and zero otherwise. If  $X$  is a set, then we denote by  $2^X$  the set of all the subsets of  $X$ ;  $|2^X| = 2^n$ . We further denote by  $\binom{X}{k}$  the set of all subsets of  $X$  of cardinality  $k$ . We have

$$\left| \binom{X}{k} \right| = \binom{n}{k} = \frac{n!}{k!(n-k)!}.$$

The *binomial theorem* says that

$$(x + y)^n = \sum_{k=0}^n \binom{n}{k} x^k y^{n-k}.$$

The symbol  $\binom{n}{k}$  is called the *binomial coefficient*. The *multinomial coefficient* is defined by

$$\binom{n}{k_1, \dots, k_m} = \frac{n!}{k_1! \cdots k_m!}$$

and the *multinomial theorem* says that

$$(x_1 + \cdots + x_m)^n = \sum_{k_1 + \cdots + k_m = n} \binom{n}{k_1, \dots, k_m} x_1^{k_1} \cdots x_m^{k_m}.$$

A very good estimate of the factorial function  $n!$  is given by Stirling's formula which approximates  $n!$  by  $(2\pi n)^{1/2} (\frac{n}{e})^n$ .

If  $Y \subset X$ , then the *incidence vector* of  $Y$  will be denoted by  $i(Y)$ ;  $i(Y)$  is the  $0,1$  vector indexed by the elements of  $X$ , where  $[i(Y)]_z = 1$  if and only if  $z \in Y$ .

We will sometimes not distinguish between a set and its incidence vector.

An *ordered pair* is usually denoted by  $(x, y)$  where  $x$  is the first element of the pair. A *binary relation* on  $X$  is any subset of  $X \times X = \{(x, x'); x \in X, x' \in X\}$ .

Any function  $X \rightarrow X$  is a binary relation on  $X$ . A *partially ordered set*, or *poset* for short, is a pair  $(X, \preceq)$ , where  $X$  is a set and  $\preceq$  is a binary relation on  $X$  that is reflexive ( $x \preceq x$ ), transitive ( $x \preceq y$  and  $y \preceq z$  imply  $x \preceq z$ ), and (weakly) antisymmetric ( $x \preceq y$  and  $y \preceq x$  imply  $x = y$ ).

The binary relation  $\preceq$  is itself called a *partial ordering*. A partial ordering where any pair of elements is comparable is called a *linear ordering*.

An important example of a linear ordering is the *lexicographic ordering*. Let  $a = (a_1, \dots, a_n)$  and  $b = (b_1, \dots, b_m)$  be two strings of integers.

We say that  $a$  is lexicographically smaller than  $b$  if  $a$  is an initial segment of  $b$  or  $a_j < b_j$  for the smallest index  $j$  such that  $a_j \neq b_j$ .

Let  $(X, \preceq)$  be a poset and  $Y \subset X$ . We say that  $Y$  is a *chain* if the induced ordering  $(Y, \preceq)$  is linear.

The symbol  $\mathbb{F}$  will denote a field;  $\mathbb{F}$  will usually be equal to  $\mathbb{R}$  or  $\mathbb{C}$ , or to the finite 2-element field  $\mathbb{GF}(2) = (\{0,1\}, +, \times)$  with addition and multiplication modulo 2.

The symbol  $\mathbb{F}^d$  denotes the vector space of dimension  $d$  over  $\mathbb{F}$ . The elements of  $\mathbb{F}^d$  are called vectors; for  $x \in \mathbb{F}^d$  we write  $x = (x_1, \dots, x_d)$ .

We will understand vectors as both row and column vectors. The scalar product of two vectors  $x, y$  is  $xy = x_1y_1 + \cdots + x_dy_d$ .

A set  $\{x^1, \dots, x^k\}$  of vectors of  $\mathbb{F}^d$  is *linearly independent* if, whenever  $\sum_{i=1}^k a_i x^i = 0$  and each  $a_i \in \mathbb{F}$ , then  $a_1 = a_2 = \cdots = a_k = 0$ .

The *dimension*  $\dim(\{x^1, \dots, x^k\})$  of a set of vectors  $\{x^1, \dots, x^k\}$  is the maximum number of linearly independent elements in  $\{x^1, \dots, x^k\}$ .

A *subspace* of a vector space  $\mathbb{F}^d$  is any subset of  $\mathbb{F}^d$  which is closed under addition, and multiplication by an element of  $\mathbb{F}$ .

Two subspaces  $X, Y$  are *isomorphic* if there is a bijection  $f: X \rightarrow Y$  such that for each  $a, b \in X$  and  $c \in \mathbb{F}$ ,  $f(a + b) = f(a) + f(b)$  and  $f(ca) = cf(a)$ .

The *orthogonal complement*

of a subspace  $X \subset \mathbb{F}^d$  is the subspace  $\{y \in \mathbb{F}^d; xy = 0 \text{ for each } x \in X\}$ .

Let  $A = (a_{ij})$  be a matrix of  $n$  rows and  $m$  columns, with entries from field  $\mathbb{F}$ . We say that  $A$  is an  $n \times m$  matrix. If  $n = m$  then  $A$  is a *square matrix*. The *determinant* of a square  $n \times n$  matrix  $A$  is defined by  $\det(A) = \sum_{\pi} (-1)^{\text{sign}(\pi)} \prod_{i=1}^n a_{\pi(i)i}$ , where the sum is over all permutations of  $1, \dots, n$  and  $\text{sign}(\pi) = |\{i < j; (\pi(i) > \pi(j))\}|$ . The determinant characterizes linearly independent vectors. A set of  $n$  vectors of length  $n$  is linearly independent if and only if  $\det(A) \neq 0$ , where  $A$  is the matrix whose set of columns (or rows) is formed by the vectors. The determinant of a matrix may be calculated efficiently by the *Gaussian elimination*. The *permanent* of matrix  $A$  is defined analogously as the determinant, but the  $(-1)^{\text{sign}(\pi)}$  term is omitted from each summand. Hence,  $\text{Per}(A) = \sum_{\pi} \prod_{i=1}^n a_{\pi(i)i}$ . There is no efficient algorithm to calculate the permanent. The *identity matrix* is the square matrix  $A$  such that  $a_{ii} = 1$  and  $a_{ij} = 0$  for  $i \neq j$ . The *trace* of a square matrix  $A$ , denoted by  $\text{tr}(A)$ , is defined by  $\text{tr}(A) = \sum_i a_{ii}$ .

The symbol  $\mathbb{R}^d$  also denotes the Euclidean space of dimension  $d$ . A *curve* in  $\mathbb{R}^d$  is the image of a continuous function  $f: [0,1] \rightarrow \mathbb{R}^d$ . A curve is *simple* if it is one-to-one, and it *connects* its endpoints  $f(0), f(1)$ . A curve is *closed* if  $f(0) = f(1)$ . The *Euclidean norm* of  $x \in \mathbb{R}^d$  is  $\|x\| = (xx)^{1/2}$ . A set  $\{x^0, x^1, \dots, x^k\}$  of vectors of  $\mathbb{R}^d$  is *affinely independent* if, whenever  $\sum_{i=0}^k a_i x^i = 0$ ,  $\sum_{i=0}^k a_i = 0$  and each  $a_i \in \mathbb{R}$ , then  $a_0 = a_1 = \dots = a_k = 0$ . For two points  $x_0, x_1$  affine independence means  $x^0 \neq x^1$ ; for three points it means that  $x^0, x^1, x^2$  do not lie on a common line; for four points it means that they do not lie on a common plane; and so on. The *rank* of a set of points of  $\mathbb{R}^d$ , denoted by  $\text{rank}(\{x^0, \dots, x^k\})$ , is the maximum number of affinely independent elements in  $\{x^0, \dots, x^k\}$ .

There is a simple relation between linear and affine independence:  $x^0, \dots, x^k$  are affinely independent if and only if  $x^1 - x^0, \dots, x^k - x^0$  are linearly independent. This happens if and only if the  $(d+1)$ -dimensional vectors  $(1, x^0), \dots, (1, x^k)$  are linearly independent. An *affine subspace* is any subset  $A \subset \mathbb{R}^d$  which contains, for each pair of its elements  $x, y$ , the line through  $x, y$ . A *hyperplane* in  $\mathbb{R}^d$  is a  $(d-1)$ -dimensional affine subspace, i.e., a set of the form  $\{x \in \mathbb{R}^d : ax = b\}$  for some nonzero  $a \in \mathbb{R}^d$  and  $b \in \mathbb{R}$ . A (closed) *half-space* has the form  $\{x \in \mathbb{R}^d : ax \leq b\}$  for some nonzero  $a \in \mathbb{R}^d$  and  $b \in \mathbb{R}$ .

A set  $C \subset \mathbb{R}^d$  is *convex* if for every  $x, y \in C$ , the segment  $\{ax + (1-a)y : 0 \leq a \leq 1\}$  between  $x$  and  $y$  is contained in  $C$ . The *convex hull* of a set  $X \subset \mathbb{R}^d$  is the intersection of all convex sets containing  $X$ , and it is denoted by  $\text{conv}(X)$ . Each  $x \in \text{conv}(X)$  may be written as a *convex combination* of elements of  $X$ : there are  $x^1, \dots, x^k \in X$  and real numbers  $a_1, \dots, a_k \geq 0$  such that  $\sum_{i=1}^k a_i = 1$  and  $x = \sum_{i=1}^k a_i x^i$ .

A *convex polytope* is the convex hull of a finite subset of  $\mathbb{R}^d$ . Each convex polytope can be expressed as the intersection of finitely many half-spaces. Conversely, by the Minkowski-Weyl theorem, if an intersection of finitely many half-spaces is bounded, then it is a convex polytope. A *face* of a convex polytope  $P$  is  $P$  itself or a non-empty intersection of  $P$  with a hyperplane that does not dissect  $P$  (i.e., not both of the open half-spaces defined by the hyperplane

intersect  $P$  in a non-empty set).

## 1.2 Algorithms and Complexity

Algorithmic considerations are important for many concepts of both discrete mathematics and statistical physics. We make only basic algorithmic remarks in this book, and therefore the following exposition on algorithms and complexity is very brief.

Informally, an *algorithm* is a set of instructions to be carried out mechanically. Applying an algorithm to its *input* we get some *output*, provided that the sequence of the instructions prescribed by applying the algorithm terminates. The application of an algorithm is often called a *computation*. Usually inputs and outputs are strings (words, finite sequences) from a finite alphabet; a basic example are binary words, i.e., finite sequences of  $0,1$ . The notion of an algorithm is usually formalized by the definition of a Turing machine.

A *Turing machine* consists of the following components:

- a finite set  $S$  called the *alphabet*,
- an element  $b \in S$  called the *blank symbol*,
- a subset  $A \subset S$  called the *external alphabet*; we assume  $b \notin A$ ,
- a finite set  $Q$  whose elements are called *states* of the Turing machine,
- an initial state  $s \in Q$ ,
- a *transition function*, i.e., a function

$$t: Q \times S \rightarrow Q \times S \times \{-1,0,1\}.$$

A Turing machine has a *tape* that is divided into cells. Each cell carries one symbol from  $S$ . We assume that the tape is infinite, thus the content of the tape is an infinite sequence  $s = s_0, s_1, \dots$  of elements of  $S$ .

A Turing machine also has a read-write *head* that moves along the tape and changes symbols. If the head is in position  $p$  along the tape, it can read symbol  $s_p$  and write another symbol in its place.

The behaviour of a Turing machine is determined by a control device. At each step of the computation, this device is in some state  $q \in Q$ . The state  $q$  and the symbol  $s_p$  under the head determine the action performed by the Turing machine: the value of the transition function,  $t(q, s_p) = (q', s', p')$ , contains the new state  $q'$ , the new symbol  $s'$  to be written in the place of  $s_p$ , and the shift  $p' \in \{-1,0,1\}$  of the position of the head. If the head bumps into the left boundary of the tape (that happens when  $p + p' < 0$ ), then the computation *stops*.

Next we describe the input given to the Turing machine, and how the output is obtained. Let  $A^*$  denote the set of all the strings (finite sequences) of elements

of  $A$ . Inputs and outputs to the Turing machine with the external alphabet  $A$  are strings from  $A^*$ . An input string  $\mathcal{I}$  is written on the tape and followed by the blank symbol  $\mathfrak{b}$ . Initially, the head is at the beginning (left end) of  $\mathcal{I}$ . If the Turing machine stops (by bumping into the left boundary of the tape), we read the tape from left to right starting from the left end until we reach some symbol that does not belong to  $A$ . The initial segment of the tape until that symbol will be the output of the Turing machine.

Every Turing machine *computes* a function from a subset of  $A^*$  to  $A^*$ . There are functions that are *not computable*. A Turing machine is obviously an algorithm in the informal sense. The converse assertion is called the

*Church-Turing thesis*: Any algorithm can be realised by a Turing machine. Note that the Church-Turing thesis is not a mathematical theorem, but rather a statement about our understanding of the informal notion of algorithm.

*Complexity classes*. The computability of a function does not guarantee that we can compute it in practice since an algorithm may require too much time. The idea of an effective algorithm is usually formalized by the notion of *polynomial algorithms*. We say that a function  $\mathcal{T}$  on the positive integers is of *polynomial growth* if  $\mathcal{T}(n) \leq cn^d$  for all  $n$  and some constants  $c, d$ . We say that a function  $\mathfrak{f}$  defined on the binary strings of  $\{0,1\}^*$  is *computable in polynomial time* if there exists a Turing machine that computes  $\mathfrak{f}$  in time  $\mathcal{T}(n)$  of polynomial growth, where  $n$  is the length of the input. Such a Turing machine is called a *polynomial algorithm*. Polynomial time *encoding* plays a crucial role. For instance, if the input is an integer  $N$  in the *unary* representation then the input size is  $|N|$  but if the representation is binary, the input size is only  $\log(|N|)$ . The class of all functions computable in polynomial time is denoted by  $\mathcal{P}$ . We should remark here that computability in polynomial time does not guarantee practical computability either, but it is a good indication for it.

A special class of algorithmic problems are the *decision problems*. In a decision problem, we want the answer to be *yes* or *no*. This clearly may be modeled as a function from a subset of  $A^*$  to  $\{0,1\}$  where 0 encodes *no* and 1 encodes *yes*. It is customary to call such functions *predicates*. One can think about predicates as about properties: the predicate indicates for each string whether it has the property (yes) or does not have the property (not). Hence the algorithmic problem to compute a predicate may be formulated as the algorithmic problem to test the corresponding property.

Another basic complexity class, the class  $\mathcal{NP}$ , is usually defined only for the predicates. We say that a predicate  $\mathcal{R}(x, y)$ , where  $x$  and  $y$  are binary strings, is *polynomially decidable* if there is a Turing machine that computes it in time of polynomial growth (the size of the input is  $|x| + |y|$ ).

The class  $\mathcal{NP}$  is the class of all predicates  $\mathfrak{f}$  for which there is a polynomial growth function  $\mathcal{T}(n)$  and a polynomially decidable predicate  $\mathcal{R}$  of two variables so that  $\mathfrak{f}(x) = 1$  if and only if there is  $y$  such that  $|y| < \mathcal{T}(|x|)$  and  $\mathcal{R}(x, y) = 1$ . Informally,  $\mathcal{NP}$  is the class of the predicates (i.e., properties), for which there is a certificate (coded by  $y$ ) that can be checked in polynomial time. Most of the properties discussed in this book belong to  $\mathcal{NP}$ .

Clearly  $\mathcal{P} \subset \mathcal{NP}$ . Over the past 30 years intensive research has been directed

towards proving that the inclusion is strict. The question whether  $P \neq NP$  is today one of the fundamental problems of both mathematics and computer science.

*Reducibility.* When can we say that one problem is algorithmically at least as hard as another problem? We model the efficiency by the polynomial time complexity, and so the answer is naturally given by the following notion of *polynomial reducibility*: we say that a predicate  $f_1$  is *polynomially reducible* to a predicate  $f_2$  if there exists a function  $g \in P$  so that  $f_1(x) = f_2(g(x))$ , for each input string  $x$ .

A predicate  $f \in NP$  is called *NP-complete* if any predicate in  $NP$  is polynomially reducible to it. The predicates that are NP-complete are the most difficult predicates of  $NP$ : if some NP-complete predicate is in  $P$  then  $P = NP$ . It is customary to speak about *NP-complete problems* rather than NP-complete predicates. The existence of an efficient algorithm to solve an NP-complete problem is considered to be very unlikely.

A seminal result in algorithmic complexity is that NP-complete predicates (problems) exist. This was proved independently by Cook and Levin. Many natural NP-complete problems are known, see [GJ].

### 1.3 Generating functions

A useful way of counting is provided by generating functions. If  $f$  is a function from the non-negative integers, we can consider its (ordinary) *generating function*  $\sum_{n \geq 0} f(n)x^n$  and its *exponential generating function*  $\sum_{n \geq 0} f(n)x^n/n!$ .

The generating functions are *formal power series*, since we are not concerned with letting  $x$  take particular values, and we ignore questions of convergence. This formalism is convenient since we can perform various operations on the formal power series, for instance

$$\left( \sum_{n \geq 0} a_n x^n \right) + \left( \sum_{n \geq 0} b_n x^n \right) = \sum_{n \geq 0} (a_n + b_n) x^n,$$

$$\left( \sum_{n \geq 0} a_n x^n / n! \right) + \left( \sum_{n \geq 0} b_n x^n / n! \right) = \sum_{n \geq 0} (a_n + b_n) x^n / n!$$

and

$$\left( \sum_{n \geq 0} a_n x^n \right) \left( \sum_{n \geq 0} b_n x^n \right) = \sum_{n \geq 0} c_n x^n$$

$$\left( \sum_{n \geq 0} a_n x^n / n! \right) \left( \sum_{n \geq 0} b_n x^n / n! \right) = \sum_{n \geq 0} d_n x^n / n!$$

where  $c_n = \sum_{i=0}^n a_i b_{n-i}$  and  $d_n = \sum_{i=0}^n \binom{n}{i} a_i b_{n-i}$ .

These operations coincide with the addition and multiplication of functions

when the power series converge for some values of  $x$ . Let us denote by  $\mathbb{C}[[x]]$  the set of all formal power series  $\sum_{n \geq 0} a_n x^n$  with complex coefficients. Addition and multiplication in  $\mathbb{C}[[x]]$  are clearly commutative, associative and distributive, thus  $\mathbb{C}[[x]]$  forms a commutative ring where 1 is the unity. Formal power series with the coefficients in a non-commutative ring (like the square matrices of the same size) are also extensively considered; they form a non-commutative ring with unity.

If  $F(x)$  and  $G(x)$  are elements of  $\mathbb{C}[[x]]$  satisfying  $F(x)G(x) = 1$  then we write  $G(x) = F(x)^{-1}$ . It is easy to see that  $F(x)^{-1}$  exists if and only if  $a_0 = F(0) \neq 0$ . If  $F(x)^{-1}$  exists then it is uniquely determined. We have  $(F(x)^{-1})^{-1} = F(x)$ .

*Example 1.3.1.* Let  $a \neq 0$  and  $(\sum_{n \geq 0} a^n x^n)(1 - ax) = \sum_{n \geq 0} c_n x^n$ , where  $a$  is a non-zero complex number. Then from the definition of multiplication we get  $c_0 = 1$  and  $c_n = 0$  for  $n > 0$ . Hence we may write

$$\sum_{n \geq 0} a^n x^n = (1 - ax)^{-1}.$$

The identity may be derived in the same way in every ring of formal power series over a (not necessarily commutative) ring with unity. Hence, for instance, for square complex matrices it can be written as

$$\sum_{n \geq 0} A^n x^n = (I - Ax)^{-1}.$$

This is of course just the formula for summing a geometric series. Informally speaking, if we have an identity involving power series that is valid when the power series are regarded as functions (when the variables are sufficiently small complex numbers), then the identity remains valid when regarded as an identity among formal power series. Formal power series may naturally have more than one variable.

## 1.4 Principle of inclusion and exclusion

Let us start with the introduction of a paper of Whitney, which appeared in *Annals of Mathematics* in August 1932:

”Suppose we have a finite set of objects (for instance books on a table), each of which either has or has not a certain given property  $A$  (say of being red). Let  $n$  be the total number of objects,  $n(A)$  the number with the property  $A$ , and  $n(\bar{A})$  the number without the property  $A$ . Then obviously  $n(\bar{A}) = n - n(A)$ . Similarly, if  $n(AB)$  denotes the number with both properties  $A$  and  $B$ , and  $n(\bar{A}\bar{B})$  the number with neither property, then  $n(\bar{A}\bar{B}) = n - n(A) - n(B) + n(AB)$ , which is easily seen to be true. The extension of these formulas to the general case where any number of properties is considered is quite simple, and is well known to logicians. It should be better known to mathematicians also; we give in this paper several applications which show its usefulness.”

It is known today, under the name *principle of inclusion and exclusion* (PIE).



**Theorem 1.4.1.** Suppose  $A_1, \dots, A_n$  are finite sets, and  $A_J = \bigcap_{i \in J} A_i$ . Then

$$\left| \bigcup_{i=1}^n A_i \right| = \sum_{k=1}^n (-1)^{k-1} \sum_{J \in \binom{[n]}{k}} |A_J|.$$

*Proof.* We proceed by induction on  $n$ . The case  $n = 2$  is clear. In the induction step,

$$\begin{aligned} \left| \bigcup_{i=1}^n A_i \right| &= \left| \bigcup_{i=1}^{n-1} A_i \cup A_n \right| = \\ |A_n| + \sum_{k=1}^{n-1} (-1)^{k-1} \sum_{J \in \binom{[n-1]}{k}} |A_J| - \left| \bigcup_{i=1}^{n-1} (A_i \cap A_n) \right| &= \\ \sum_{k=1}^n (-1)^{k-1} \sum_{J \in \binom{[n]}{k}} |A_J|. \end{aligned}$$

□

Let  $(X, \leq)$  be a finite partially ordered set (poset). For example, the set of all subsets of a finite set  $S$  equipped with the relation ' $\subset$ ' forms a poset called the *Boolean lattice*. Let  $\mathbb{F}$  be a field and let us denote by  $\mathcal{F}(X)$  the collection of all functions  $f : X \times X \rightarrow \mathbb{F}$ , with the property that  $f(x, y) \neq 0$  only if  $x \leq y$ . We equip the set  $\mathcal{F}(X)$  with the *convolution product*

$$(f * g)(x, y) = \sum_{x \leq z \leq y} f(x, z)g(z, y).$$

It is straightforward to verify that the convolution product is associative.

We recall from the introduction that the *Kronecker delta function* is defined by  $\delta(x, y) = 1$  if and only if  $x = y$ , and it is zero otherwise. The Kronecker delta function acts as the identity function with respect to the convolution product, since  $\delta * f = f * \delta = f$ . Another basic function is the *zeta function* defined by  $\zeta(x, y) = 1$  if  $x \leq y$ , and  $\zeta(x, y) = 0$  otherwise.

**Theorem 1.4.2.** Let  $f \in \mathcal{F}(X)$  be a function such that  $f(x, x) \neq 0$  for each  $x \in X$ . Then there is unique function  $g$  so that  $f * g = g * f = \delta$ .

*Proof.* We can define  $g$  inductively by first letting

$$g(x, x) = 1/f(x, x),$$

and then letting

$$g(x, y) = - \sum_{x \leq z < y} g(x, z) \frac{f(z, y)}{f(y, y)}.$$

Hence  $g * f = \delta$  and so  $g$  is the *left inverse* of  $f$ . Similarly we can define function  $h$  which is the *right inverse* of  $f$ . By associativity,  $g = g * \delta = g * (f * h) = (g * f) * h = \delta * h = h$ .

□

Another basic function is the inverse of the zeta function; it is called the *Möbius function* and denoted by  $\mu(x, y)$ . We immediately have

*Exercise 1.4.3.*  $\mu(x, x) = 1$  and  $\mu(x, y) = -\sum_{x \leq z < y} \mu(x, z)$ .

*Exercise 1.4.4.* Prove by induction on  $|B - A|$  that the Möbius function of the Boolean poset  $(2^n, \subset)$  is given by  $\mu(A, B) = (-1)^{|B-A|}$ .

*Exercise 1.4.5.* Let  $(X, \leq)$  be an interval in the set of integers. Then  $\mu(x, x) = 1$ ,  $\mu(x, x+1) = -1$  and  $\mu(x, y) = 0$  otherwise.

Let us state the *Möbius inversion formula* (MIF).

**Theorem 1.4.6.** Let  $(X, \leq)$  be a finite poset and let  $f, g$  be two functions from  $X$  to  $\mathbb{F}$ . Then  $g(x) = \sum_{y \leq x} f(y)$  for all  $x \in X$  if and only if  $f(x) = \sum_{y \leq x} g(y)\mu(y, x)$  for all  $x \in X$ .

*Proof.*

$$\begin{aligned} \sum_{y \leq x} g(y)\mu(y, x) &= \sum_{y \leq x} \sum_{z \leq y} f(z)\mu(y, x) = \\ &= \sum_{y \leq x} \mu(y, x) \sum_{z \in X} (z, y)f(z) = \\ &= \sum_{z \in X} \left( \sum_{z \leq y \leq x} (z, y)\mu(y, x) \right) f(z) = \\ &= \sum_{z \in X} (z, x)f(z) = f(x). \end{aligned}$$

□

If  $(X, \leq_1)$  and  $(Y, \leq_2)$  are two posets then their *direct product* is the poset  $(Z, \leq)$  where  $Z = X \times Y = \{(x, y); x \in X, y \in Y\}$  and  $(x, y) \leq (x', y')$  if  $x \leq_1 x'$  and  $y \leq_2 y'$ .

**Theorem 1.4.7.** The Möbius function of the direct product of two posets is the product of their Möbius functions:  $\mu((x_1, y_1)(x_2, y_2)) = \mu_1(x_1, x_2)\mu_2(y_1, y_2)$ .

*Proof.* This can be proven in a straightforward way by induction on the number of pairs  $(u, v)$  that lie between  $(x, y)$  and  $(x', y')$ , and using Exercise 1.4.3. □

The following theorem is an easy consequence of Exercise 1.4.3.

**Theorem 1.4.8.** Let  $P$  be a finite poset and let  $P'$  be  $P$  with adjoined smallest and largest elements (denoted by  $0$  and  $1$ ). Let  $c_i$  be the number of chains in  $P'$  between  $0, 1$  of length  $i$ . Then  $\mu(0, 1) = c_0 - c_1 + \dots$ .

This means that  $\mu(0, 1)$  may be interpreted as the *Euler characteristic* of the abstract simplicial complex associated with  $P'$  (see Section 5.1).

Applying Theorem 1.4.6 to the Boolean lattice, and using Exercise 1.4.4, we get

**Corollary 1.4.9.** Let  $F$  be a function on the set  $2^S$  of all subsets of an  $n$ -element set  $S$  to a field  $\mathbb{F}$ . For  $K \subset S$  let  $G(K) = \sum_{L \subset K} F(L)$ . Then

$$F(K) = \sum_{L \subset K} (-1)^{|K-L|} G(L).$$

Corollary 1.4.9 implies a formula which gives a simple exponential algorithm to calculate a permanent.

**Corollary 1.4.10.** Let  $A$  be an  $n \times n$  matrix. Then

$$\text{Per} A = \sum_{S \subset \{1, \dots, n\}} (-1)^{n-|S|} \prod_{i=1}^n \left( \sum_{j \in S} a_{ij} \right).$$

Next we consider the poset  $(X, \preceq)$  where  $X = \{1, 2, \dots, n\}$  and  $a \preceq b$  if  $a$  divides  $b$ .

**Theorem 1.4.11.** Let  $\mu$  be the Möbius function of  $(X, \preceq)$ . Then  $\mu(1, 1) = 1$ ,  $\mu(k, n) = \mu(1, \frac{n}{k})$  if  $k$  divides  $n$ ,  $\mu(1, n) = (-1)^m$  if  $n$  is a product of  $m$  distinct primes, and  $\mu(1, n) = 0$  otherwise.

*Proof.* The first claim is simple. For the second one let  $n = p_1^{\alpha_1} \cdots p_k^{\alpha_k}$  be the unique factorization of  $n$  into primes. Clearly, we only need to consider the Möbius function of  $(X', \preceq)$ , where  $X'$  consists of all positive integers that divide  $n$ . Clearly,  $(X', \preceq)$  is the direct product of the linearly ordered sets  $(X_i, \preceq)$ ,  $i = 1, \dots, k$ , where  $X_i = \{1, p_i, \dots, p_i^{\alpha_i}\}$ . The theorem thus follows from Theorem 1.4.7 and Exercise 1.4.5.  $\square$

The Euler function  $\phi(n)$  is equal to the number of integers  $1 \leq k \leq n$  such that  $k$  and  $n$  have the greatest common divisor equal to 1. For example  $\phi(9) = 6$ . A classical formula that precedes all general Möbius inversion formulas reads as follows.

**Theorem 1.4.12.**

$$\phi(n) = n \prod_{p|n} (1 - 1/p),$$

where the product is over all distinct primes  $p$  dividing  $n$ .

*Proof.* Let  $d$  divide  $n$ . Then  $\sum_{d|k} \mu(k, d)$  equals the number of integers  $1 \leq k \leq n$  such that the greatest common divisor of  $k, n$  is  $d$ , since any such integer  $k$  is of the form  $k = dk'$  where  $1 \leq k' \leq \frac{n}{d}$  and the greatest common divisor of  $k'$  and  $\frac{n}{d}$  is 1.

We take the function  $f$  in the Möbius inversion formula 1.4.6 to be the Euler function  $\phi$ . Let  $g(x) = \sum_{y \preceq x} f(y)$ . We observe that  $g(n) = n$ , since for each  $1 \leq k \leq n$  there is unique  $d$  such that the greatest common divisor of  $k$  and  $n$  is  $d$ . The inversion formula and Theorem 1.4.11 thus give

$$\phi(n) = \sum_{d \preceq n} \mu(d, n) d = \sum_{d \preceq n} \mu(1, d) \frac{n}{d}.$$

Let  $p_1, \dots, p_k$  be the distinct primes that divide  $n$ . Theorem 1.4.11 gives

$$\begin{aligned} (n) &= n - \left( \frac{n}{p_1} + \frac{n}{p_2} + \dots \right) + \left( \frac{n}{p_1 p_2} + \frac{n}{p_1 p_3} + \dots \right) - \dots = \\ & n \prod_{i=1}^k \left( 1 - \frac{1}{p_i} \right). \end{aligned}$$

□



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## Chapter 2

# Introduction to Graph Theory

### 2.1 Basic notions of graph theory

A graph is an ordered pair of sets  $(V, E)$  such that  $E$  is a subset of the set  $\binom{V}{2}$  of unordered pairs of elements of  $V$ . The set  $V = V(G)$  is the set of *vertices* and  $E = E(G)$  is the set of *edges*. The vertices  $u$  and  $v$  are the *endvertices* of this edge and we also say that  $u, v$  are *adjacent* vertices in  $G$ .

We say that  $G' = (V', E')$  is a *subgraph* of  $G = (V, E)$  if  $V' \subset V$  and  $E' \subset E$ . If a subgraph  $G'$  contains all the edges induced by a subset  $V'$  of vertices, then  $G'$  is called an *induced subgraph*. If  $V' = V$  then  $G'$  is a *spanning subgraph*. If  $V' \subset V$  then  $G - V'$  is the subgraph of  $G$  induced by  $V \setminus V'$ . If  $E' \subset E$  then  $G - E' = (V, E \setminus E')$ . If  $V' = \{v\}$  and  $E' = \{e\}$  then we may write  $G - v, G - e$  instead of  $G - V', G - E'$ . Two graphs are *isomorphic* if one may be obtained from the other by renaming the vertices. The *degree*  $\deg_G(v)$  of a vertex  $v$  is equal to the number of vertices incident with  $v$ . Clearly, the sum of all the degrees equals twice the number of edges of the graph. A subset  $E' \subset E$  of edges is called *even* if the graph  $(V, E')$  has all degrees even (zero is an even number).

A *walk* in a graph is a sequence  $v_1, e_1, v_2, e_2, \dots, v_i, e_i, v_{i+1}, \dots, e_n, v_{n+1}$  such that each  $v_j$  is a vertex and each  $e_j = v_j v_{j+1}$  is an edge. The vertices  $v_1$  and  $v_{n+1}$  are the endvertices of the walk and  $n$  is its length. A walk is called a *trail* if all of its edges are distinct, and a *path* if all of its vertices are distinct. Hence a path is necessarily a trail. A walk whose endvertices coincide is called a *closed walk*. The set of the edges of a path whose endvertices coincide is called a *cycle*. A cycle which induces an induced subgraph on its vertices is *induced cycle*.

A graph  $G = (V, E)$  is *connected* if it has a path between any pair of vertices. If a graph is not connected, then it is naturally partitioned into maximal connected *components*.

We will use the symbol  $P_n$  to denote a path of length  $n$ , and  $C_n$  to denote a

cycle of length  $n$ . Moreover,  $K_n$  denotes a *complete graph* with  $n$  vertices and all possible edges. Hence  $K_n$  has  $\binom{n}{2}$  edges.

A graph  $G$  is a *bipartite graph* if  $V$  may be partitioned into vertex classes (or parts)  $V_1$  and  $V_2$ , i.e.  $V = V_1 \cup V_2$  and  $V_1, V_2$  are disjoint, such that every edge joins a vertex of  $V_1$  to a vertex of  $V_2$ :

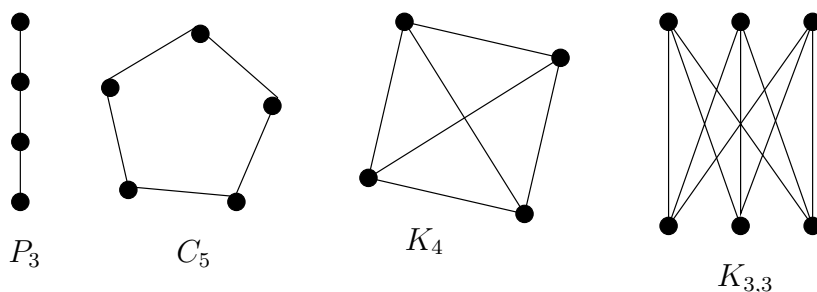
$$E \subset \{\{v_1, v_2\}; v_1 \in V_1, v_2 \in V_2\}.$$

We denote by  $K_{m,n}$  the complete bipartite graph whose vertex classes have  $m$  and  $n$  vertices. It is not difficult to make the following observation.

**Observation 2.1.1.** *A graph  $G$  is bipartite if and only if it has no cycle of odd length.*

*Proof.* A subgraph of a bipartite graph is bipartite and no cycle of an odd length is bipartite. This shows the only if part. On the other hand, if  $G$  has no cycle of odd length then the following 'greedy' algorithm finds the bipartition of each component: color an arbitrary vertex by 1, all its neighbours by 2, all their neighbours by 1 and so on.  $\square$

A very natural way to describe a graph is to draw it. Figure 2.1 illustrates the basic graphs by pictures.



**Figure 2.1.** Basic pictures of graph theory

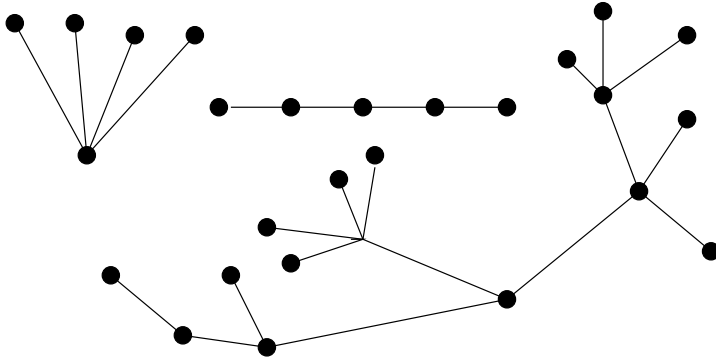
A graph with no cycle is a *forest* or an *acyclic graph*. A *tree* is a connected forest. Clearly each forest is bipartite.

**Observation 2.1.2.** *Each tree with at least one edge has at least two vertices of degree one.*

*Proof.* The endvertices of any maximal path in the tree are vertices of degree one.  $\square$

A vertex of degree one in a tree is called a *leaf*.

**Observation 2.1.3.** *For a graph  $G = (V, E)$ , the following statements are equivalent:*



**Figure 2.2.** Examples of trees

- (1)  $G$  is a tree,
- (2)  $G$  is connected and becomes disconnected after deletion of any edge ( $G$  is a minimal connected graph),
- (3)  $G$  is a maximal acyclic graph,
- (4)  $G$  is connected and  $|E| = |V| - 1$ .

*Proof.* All four properties are invariant under deleting or adding a vertex of degree one. We know by Observation 2.1.2 that a tree has a vertex of degree one, so in order to prove the observation by induction on the number of vertices of  $G$  it suffices to show that the graphs which satisfy the second or the third or the fourth property must have a vertex of degree one: if  $G$  satisfies (2) or (3) then it cannot have a cycle and hence it must have a vertex of degree one by the same argument which proves Observation 2.1.2. If  $G$  satisfies (4) then it must have a vertex of degree one since the sum of the degrees equals  $2|E|$ .  $\square$

A tree which is a subgraph of a graph  $G$  will be called a *subtree* of  $G$ . A subtree is called a *spanning tree* if it contains all vertices of the graph. Similarly a *spanning forest* of a graph is a subforest which contains all vertices. It follows from Observation 2.1.3 that every connected graph has a spanning tree, and every graph has a spanning forest.

If a graph  $G$  is connected, and for some set  $U$  of vertices  $G - U$  is disconnected, then we say that  $U$  *separates*  $G$ , or that  $U$  is a *vertex cut*, or simply a *cut*. If vertices  $s, t$  belong to different components of  $G - U$ , then we say that  $U$  separates  $s$  from  $t$ . A vertex that separates  $G$  is called a *cutvertex*. For  $k \geq 2$ , we say that  $G$  is  *$k$ -connected* if either  $G$  is a complete graph  $K_{k+1}$  or it has at least  $k + 2$  vertices and no set of  $k - 1$  vertices separates it.

Similarly we can say that a set  $E'$  of edges separates a graph  $G$  if  $G - E'$  is disconnected. An edge that separates  $G$  is called a *bridge* of  $G$ . A graph is  *$k$ -edge-connected* if it has at least two vertices and no set of at most  $k - 1$  edges that



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