Chapter 1

Algorithms

The term “computer” used to be a job description for a person doing the same tedious computations over and over, hopefully without error. When electrical computers became available, these human computers often transitioned to become computer programmers. Instead of doing the computations themselves, they told the computer what to do.

Definition 1.1 (Algorithm). An algorithm is a sequence of computational instructions that solves a class of problems. Often the algorithm computes an output for a given input, i.e., a mathematical function.

Remarks:  
• While the number of algorithms is theoretically unlimited, surprisingly many problems can be solved with just a few algorithmic paradigms that we will review in this chapter. A simple yet powerful algorithmic concept is recursion. Let us start with an example.

1.1 Recursion

You have won an all-you-can-carry run through an electronics store. The rules are simple: Whatever you manage to carry, you can have for free. Being well-prepared you bring a high-capacity backpack to the event. Which items should you put into your backpack such that you can carry the maximum possible value out of the store?

Problem 1.2 (Knapsack). An item is an object that has a name, a weight and a value. Given a list of items and a knapsack with a weight capacity, what is the maximal value that can be packed into the knapsack?

Remarks:  
• An algorithm solving Knapsack computes a function; the inputs are the set of possible items and the capacity limit of the knapsack, the output is the maximal possible value.
• A simple way to solve Knapsack is to check for every item whether it should be packed into the knapsack or not, expressed as the following recursion:

Algorithm 1.3: A recursive solution to Knapsack.

```python
def knapsack(items, capacity):
    if len(items) == 0:
        return 0
    first, *rest = items
    take = 0
    if first.weight <= capacity:
        take = knapsack(rest, capacity-first.weight) + first.value
    skip = knapsack(rest, capacity)
    return max(take, skip)
```

Remarks:  
• Algorithm 1.3 may look like pseudo-code, but really is correct Python.
• In Lines 7 and 8, the algorithm calls itself. This is called a recursion.

Definition 1.4 (Recursion). An algorithm that splits up a problem into sub-problems and invokes itself on the sub-problem is called a recursive algorithm. A recursion ends when reaching a simple base case that can be solved directly. Also, see Definition 1.4.

Remarks:  
• In mathematics, we find a similar structure in some prominent inductive functions such as the Fibonacci function.
• Recursive algorithms are often easy to comprehend, but not necessarily fast.
• How can we measure “fast”?

Definition 1.5 (Time Complexity). The time complexity of an algorithm is the number of basic arithmetic operations (+, −, ×, ÷, etc.) performed by the algorithm with respect to the size n of the given input.

Remarks:  
• Each variable assignment, if statement, iteration of a for loop, comparison (==, <, >, etc.) or return statement also counts as one basic arithmetic operation, and so do function calls (len(), max(), knapsack()).
• Unfortunately, there is no agreement on how the size of the input should be measured. Often the input size n is the number of input items. If input items get large themselves (e.g., the input may be a single but huge number), n refers to the number of bits needed to represent the input.
• We are usually satisfied if we know an approximate and asymptotic time complexity. The time complexity should be a simple function of \( n \), just expressing the biggest term as \( n \) goes to infinity, ignoring constant factors. Such an asymptotic time complexity can be expressed by the “big \( O \)” notation.

**Definition 1.6 (\( O \)-notation).** The \( O \)-notation is used to denote a set of functions with similar asymptotic growth. More precisely,

\[
O(f(n)) = \left\{ g(n) \mid \lim_{n \to \infty} \frac{g(n)}{f(n)} < \infty \right\}.
\]

Remarks:
- In other words, \( O(f(n)) \) is the set of functions \( g(n) \) that asymptotically do not grow much faster than \( f(n) \).
- For example, \( O(1) \) includes all constants and \( O(n) \) means “linear in the input size \( n \)”.
- In other words, the \( O \)-notation is quite crude, but nevertheless useful, both in theory and practice.
- Other useful asymptotic notations are \( \Omega() \) for lower bounds, but also \( o(1), \omega(1), \Theta(1), \) etc.

**Lemma 1.7.** The time complexity of Algorithm 1.3 is \( O(2^n) \).

Proof. Each call of the \texttt{knapsack()} -procedure performs constantly many basic arithmetic operations itself and makes (at most) two additional calls to the \texttt{knapsack()} -procedure. Hence, it suffices to count the total number of \texttt{knapsack()}-invocations. We get 1 invocation on the first item, at most 2 on the second, 4 on the third, \ldots, and \( 2^{n-1} \) on the last. Hence, there are less than \( 2^n \) invocations of the \texttt{knapsack()} -function. \( \square \)

Remarks:
- The time complexity of Algorithm 1.3 is exponential in the number of items. Even if there were only \( n = 100 \) items to be evaluated, the currently fastest supercomputer in the world would take \( 2^{100} \text{ ops}/(148 \cdot 10^{15} \text{ ops/s}) \approx 271000 \text{ years} \) to compute our \texttt{knapsack()} function. So for many realistic inputs, Algorithm 1.3 is not usable. We need a better approach!

### 1.2 Greedy

What about sorting all the items by their value-to-weight ratio, and then simply greedily packing them??
1.4. DYNAMIC PROGRAMMING

 Remarks:
• Note that Algorithm 1.12 is not correct Python. Line 3 is just pseudo-code, far from actual Python notation. Line 4 could be Python, but unfortunately needs an extra enumerate() function.
• Line 6 is incorrect: If item.weight > c, c-item.weight becomes negative. The programmer of Algorithm 1.12 assumed that accessing a negative index of an array returns 0; however, most programming languages return an error. We can fix Line 6 by adding the conditional expression if c >= item.weight else 0 to the second term of the max() function.
• The time complexity of Algorithm 1.12 is \( O(n \cdot \text{capacity}) \). In Definition 1.5 we postulated that the time complexity should be a function of \( n \). So the DP approach only makes sense when capacity is a natural number with capacity < \( 2^n/n \).

 Definition 1.13 (Space Complexity), The space complexity of an algorithm is the amount of memory required by the algorithm, with respect to the size \( n \) of the given input.

 Remarks:
• As for Definition 1.5, we are usually satisfied if we know the approximate (asymptotic) space complexity.
• Also, the amount of memory can be measured in bits or memory cells.
• The space complexity of Algorithm 1.12 is \( O(n \cdot \text{capacity}) \).
• For reasonably small capacity, Algorithm 1.12 is faster than Algorithms 1.3–1.10, but is it correct?

 Lemma 1.14. Assuming that all items have integer weights, Algorithm 1.12 solves Knapsack correctly.

 Proof. We show the correctness of each entry in the matrix \( V \) by induction. As a base case, we have \( V[0] = [0, \ldots, 0] \) since without item, no value larger than 0 can be achieved. For the induction step, assume that \( V[i] \) correctly contains the maximum values that can be achieved using only the first \( i \) items. When we set a value \( V[i+1][c] \), we can either include the item \( i \)+1 or select the optimal solution for Knapsack with capacity using only the first \( i \) items. Algorithm 1.12 stores the \( \max() \) of these two values in \( V[i+1][c] \) (for all \( c \in [0, \ldots, \text{capacity}] \)), which is thus optimal. Hence, the value \( V[n][\text{capacity}] \) contains the maximum value that can be achieved with the weight capacity, using any combination of the \( n \) items.
Top-down DP is inheriting the best of recursion and bottom-up DP. Consequentially, the time complexity of Algorithm 1.16 is $O(n \cdot \min(2^n, n \cdot \text{capacity}))$.

So far we have learned a family of related algorithmic techniques: recursion, backtracking, dynamic programming, and memoization. Together, this family can help solving many demanding algorithmic problems.

However, there are powerful algorithmic paradigms beyond this family of techniques, for instance linear programming.

### 1.5 Linear Programming

So far, we were only considering unsplittable items. However, for liquid goods, Knapsack can be solved quickly using a greedy method (Algorithm 1.8). What if we had more than one constraint?

**Problem 1.17 (Liquid Knapsack)**. A beverage has a name, a value per liter $\rightarrow$ notebook and a preparation time per liter. Given 1 hours to prepare for a party and a fridge with a storage capacity, what is the maximal value that can be prepared and stored in the fridge?

**Remarks:**

- With more than one constraint, the greedy method does not work.
- However, this problem has a nice property: the objective and the constraints are linear functions of the quantity of each prepared beverage.

We call such problems linear programs.

**Definition 1.18 (Linear Program or LP)**. A linear program (LP) is an optimization problem with $n$ variables and $m$ linear inequalities

$$a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n \leq b_1$$
$$a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n \leq b_2$$
$$\vdots \quad \vdots \quad \vdots$$
$$a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n \leq b_m$$

We are interested in finding a point $x = (x_1, \ldots, x_n)^T$ with $x_i \geq 0$ respecting all these constraints and maximizing a linear function

$$f(x) = c_1x_1 + c_2x_2 + \cdots + c_nx_n$$

where $a_{ij}$, $b_i$, and $c_i$ are given real-valued parameters. We call the point $x$ an optimum of the LP.
CHAPTER 1. ALGORITHMS

Remarks:

• There is also a short hand notation using linear algebra
  \[ \max \{ c^T x \mid Ax \leq b, x \geq 0 \}, \]
  where \( A \) is the matrix with entries \( a_{ij} \) and \( b \) and \( c \) the vectors given by the \( b_i \) and \( c_i \), respectively.

• In general, if you have the problem of maximizing or minimizing a linear function under constraints that are linear inequalities, there is a way to formulate it in the above canonical form. For instance, a constraint \( a^T x = b \) can be rewritten as a combination of \( a^T x \leq b \) and \( a^T x \geq b \) which itself can be rewritten as \( -a^T x \leq -b \). Also, minimizing a linear function with coefficients \( c_1, \ldots, c_n \) is the same as maximizing a linear function with coefficients \( -c_1, \ldots, -c_n \).

• It is possible to model some functions which do not look linear at first sight. For example, minimizing an objective function \( f(x) = |x| \) can be expressed as \( \min \{ t(x \leq 1, -x \leq 1) \} \).

Definition 1.19 (Feasible Point). Given an LP, a point is feasible if it is a solution of the set of constraints.

Remarks:

• Geometrically, the set of feasible points of an LP corresponds to an \( n \)-dimensional convex polytope. The hyperplanes bounding the polytope are given by the restricting inequalities.

• Polytopes are a generalization of 2D polygons to an arbitrary number of dimensions. Convexity, however, deserves a more formal definition.

Definition 1.20 (Convex Set). A set of points in \( \mathbb{R}^n \) is convex if for any two points of the set, the line segment joining them is also entirely included in the set.

Lemma 1.21. The set of feasible points of an LP is convex.

Proof. Given two feasible points \( x_1 \) and \( x_2 \), any point in the line segment joining them can be written as \( x = \lambda x_1 + (1 - \lambda) x_2 \) for \( \lambda \in [0, 1] \). For any constraint \( a^T x \leq b \), we compute
  \[ a^T [x_1 + \lambda(x_2 - x_1)] = (1 - \lambda)a^T x_1 + \lambda a^T x_2 \leq (1 - \lambda)b + \lambda b = b. \]

Definition 1.22. Given an LP, we call polytope the set of feasible points.

A constraint \( a^T x \leq b \) is tight at \( x \) if \( a^T x = b \). For an LP with \( n \) variables, feasible points activating \( n \) (resp. \( n - 1 \)) linearly independent constraints are called the nodes (resp. edges) of the polytope. Each edge links two nodes \( x_1, x_2 \) with \( n - 1 \) common activating constraints; we say that the two nodes \( x_1, x_2 \) are neighbors.

1.5. LINEAR PROGRAMMING

Remarks:

• A polytope can be unbounded, i.e. infinitely large. In some cases, it is even possible to have an infinitely large solution, e.g. \( \max \{ x \mid x \geq 0 \} \). Following our definition, the LP does not admit an optimum in this case.

• In order to solve an LP, one has to find a point in the polytope that maximizes our objective function \( f(x) \).

Theorem 1.23. If the polytope of an LP is bounded, then at least one node \( \rightarrow \) notebook of the polytope is an optimum of the LP.

Proof. For any value \( y \) that the objective function can take, the set of points reaching this value is given by the hyperplane \( c^T x = y \). We can find an optimum of the LP by sliding this hyperplane until the boundary of the polytope is reached, which happens at some node of the polytope.

Remarks:

• One popular method exploiting Theorem 1.23 for solving LPs is the simplex algorithm. The idea is simple: starting from a node of the LP polytope, greedily jump to a neighboring node having a better objective until you cannot improve the solution anymore.

Algorithm 1.24: Simplex Algorithm.

Remarks:

• While the simplex algorithm performs well in practice, there are instances where its time complexity is exponential in the size of the input. Other LP algorithms known as interior point methods are provably fast.

• In practice, we do not build and store the whole polytope of the LP, as the polytope could have an exponential number of nodes! Instead, we represent a node as a set of tight constraints. To find its neighbors, we remove a constraint of the set, add another constraint and check if the point is feasible.

• The node returned by the simplex algorithm is better than any neighboring node by construction, but how can we convince ourselves that no other point anywhere in the feasible polytope is better?

Definition 1.25 (Local Optimum). A feasible node \( x \) is a local optimum if \( f(x) \geq f(y) \) for any neighboring node \( y \).
Remarks:

• In contrast to a local optimum, an optimum (from Definition 1.18) is called global optimum.
• While it is easy to find a local optimum, finding a global optimum is often difficult. However, it turns out that every local optimum of an LP is also a global optimum!

Theorem 1.26. The node $x^*$ returned by the simplex algorithm is an optimum.

Proof. Let us consider the hyperplane $c^Tx = f^*$, where $f^* = c^Tx^*$. We know that all the neighbors of node $x^*$ are on the side $c^Tx \leq f^*$. Since the polytope is convex, we know that the whole polytope must be on this side of the hyperplane. Hence no node $x'$ in the polytope can be on the side $c^Tx > f^*$; and hence the node $x^*$ is a global optimum.

![Figure 1.27: Illustration of Theorem 1.26. The neighbors of $x^*$ are $x_1$ and $x_2$.](image)

Example 1.29. The following functions are convex:

- $f(x) = x^2$
- $f(x) = \|x\|_2$ (Euclidean norm)
- $f(p_1, \ldots, p_k) = \sum p_i \log p_i$ (reverse entropy)
- $f(A) = -\log \det(A)$ for a positive semidefinite matrix $A$

1.5. LINEAR PROGRAMMING

Definition 1.30 (Phase 1 LP). Given an LP

$$\max \{ c^Tx \mid Ax \leq b, x \geq 0 \},$$

we build the so-called phase 1 LP by replacing every constraint $a_i^T x \leq b_i$ with $a_i^T x - y_i \leq b_i$, introducing a new artificial variable $y_i$. If we minimize all artificial variables $y_i$, we get:

$$\max \{ -y^T \mid Ax - y \leq b, y \geq 0 \}.$$

Lemma 1.31. Setting each $x_i = 0$ and each $y_i = \max(0, -b_i)$ yields a feasible node of the phase 1 LP.

Proof. With each original variable $x_i = 0$, each constraint is reduced to $-y_i \leq b_i$, which is satisfied when $y_i = \max(0, -b_i)$.

Also, this point is a node of the polytope. Algebraically, a point is a node if at least $n$ linearly independent constraints are tight at this point. The constraint $x_i \geq 0$ is tight for each original variable $x_i$, and either $a_i x - y_i \leq b_i$ or $y_i \geq 0$ is tight for each artificial variable $y_i$, depending on the sign of $b_i$. Thus, the number of tight constraints is at least equal to the number of variables, and this point is a node of the polytope.

Lemma 1.32. If the original LP is feasible, then the phase 1 LP will find a feasible node.

Proof. If the original LP is feasible, then its polytope is not empty, i.e., there exists a feasible node $x$ in the original LP. Together with $y = 0$, node $x$ is also feasible in the phase 1 LP. Since $\max \{ -y^T \} = \min \{ \text{sum}(y) \}$ is optimal for $y = 0$, node $x$ is optimal in the phase 1 LP. With Theorem 1.26, we know that the phase 1 LP will find such a node $x$.

Algorithm 1.33: Two-phase simplex algorithm to solve LPs.

Remarks:

• Algorithm 1.33 is the complete procedure to solve an LP. This process is often called the two-phase simplex algorithm.
• In Python, one can solve an LP using the function linprog from the module scipy.optimize.

```python
def solveLP(A, b, c):
    x, y = simplex(polytope([A -I], b, 1, (0, 0, max(0,-b))))
    if sum(y) == 0:
        return simplex(polytope(A, b, c, x))
    else:
        return "no solution"
```
1.6 Linear Relaxation

Despite linear programming covering a broad class of problems, we are often confronted with discrete tasks. In practice we often need an integer solution.

Definition 1.34 (Integer Linear Programming or ILP). An integer linear program (ILP) is an LP in which all variables are restricted to integers.

Remarks:
- In a lot of combinatorial problems, variables are restricted to just two values \{0, 1\}. Such variables are called indicator ("to be or not to be") variables. We call such programs binary ILPs.
- Apart from LP and ILP, there exist many other optimization techniques: Mixed Integer Linear Programming (MILP) with both integer and continuous variables, Quadratic Programming (QP), and continuous variables, Quadratic Programming (QP), Semidefinite Programming (SDP), . . .

Problem 1.35 (ILP Knapsack). We can model Knapsack (Problem 1.2) with capacity c and n items of value \(v_i\) and weight \(w_i\) as a binary ILP, using indicator variables \(x_i\):

\[
\begin{align*}
\text{maximize} & \quad \sum v_i x_i \\
\text{subject to} & \quad \sum w_i x_i \leq c \\
& \quad x_i \in \{0, 1\}.
\end{align*}
\]

Remarks:
- Unlike LPs, no efficient algorithm solving ILPs is known.
- It is tempting to relax the constraints \(x_i \in \{0, 1\}\) to \(0 \leq x_i \leq 1\). Apply the simplex algorithm, and round the possible solution to the nearest feasible point.

Definition 1.36 (Linear Relaxation). Given a binary ILP, we construct the linear relaxation of the LP by replacing the constraint \(x_i \in \{0, 1\}\) with the constraint \(0 \leq x_i \leq 1\).

Remarks:
- However, in general, there is no guarantee that a linear relaxation finds the optimum.
- In the case of Knapsack, the solution of the linear relaxation is similar to Algorithm 1.8. All items \(i\) with a high value-to-weight ratio will get an indicator variable \(x_i = 1\), all items with a low value-to-weight ratio will get an indicator variable \(x_i = 0\). The critical item(s) in the middle will get a non-integer indicator variable which we must round down to 0 to get a valid solution. This solution can be arbitrarily bad, as the best (highest value-to-weight ratio) item might already be too heavy; we might end up without any object in the knapsack.

1.7 Flows

- However, a linear relaxation sometimes has the same optimum as its ILP. In particular, this is for some class of constraint matrices, the so-called totally unimodular matrices.
- A matrix is totally unimodular if every square submatrix has determinant −1, 0 or +1.

Problem 1.37 (Assignment Problem). Given a list of customers and a list of cabs, how to match customers to cabs in order to minimize the total waiting time?

Algorithm 1.38. This problem can be modeled as an ILP. We denote the waiting time of customer \(i\) for cab \(j\) by \(w_{ij}\). Also, we introduce a set of indicator variables \(x_{ij}\), describing the assignment: \(x_{ij} = 1\) if and only if customer \(i\) is assigned to cab \(j\). We get:

\[
\begin{align*}
\text{minimize} & \quad \sum w_{ij} x_{ij} \\
\text{subject to} & \quad \sum_j x_{ij} = 1 \quad \text{for each customer} \ i \\
& \quad \sum_i x_{ij} \leq 1 \quad \text{for each cab} \ j \\
& \quad x_{ij} \in \{0, 1\}.
\end{align*}
\]

This ILP can be solved optimally with linear relaxation: the constraint matrix is totally unimodular.

1.7 Flows

Graphs and flows are useful algorithmic concepts, related to LPs and linear relaxations.

Definition 1.39 (Graph). A graph \(G = (V, E)\) is a pair \((V, E)\), where \(V\) is a set of nodes and \(E \subseteq V \times V\) is a set of edges between the nodes. The number of nodes is denoted by \(n\) and the number of edges by \(m\).

Remarks:
- A directed graph \(G = (V, E)\) is a graph, where each edge has a direction, i.e., we distinguish between edges \((u, v)\) and \((v, u)\). If all edges of a graph are undirected, then the graph is called undirected.
- In a directed graph, we note \(\text{in}(u)\) (resp. \(\text{out}(u)\)) the set of edges entering (resp. leaving) node \(u\).
- A weighted graph \(G = (V, E, \omega)\) is a graph, where \(\omega : E \to \mathbb{R}\) assigns a weight \(\omega(e)\) for each edge \(e \in E\).
- Weights can for instance be used for delay \(d(e)\) or capacity \(c(e)\) of an edge.
- In the rest of this chapter, we consider capacitated directed graphs.
- Consider a company that wants to optimize the flow of goods in a transportation network from their factory to a customer.
Definition 1.40 (Flow). Formally, an s-t-flow from a source node s to a target
node t is given as a function \( f : E \rightarrow \mathbb{R} \) such that
\[
f(u, v) \leq c(u, v) \quad \text{for all } (u, v) \in E \quad \text{(capacity constraints)}
\]
\[
\sum_{e \in \delta(u)} f(e) = \sum_{e \in \delta(u)} f(e) \quad \text{for all } u \in V \setminus \{s, t\} \quad \text{(flow conservation)}
\]
We call the total flow reaching t the \textbf{value} of \( f \), i.e.
\[
|f| = \sum_{v \in \delta(t)} f(u, v) = \sum_{v \in \delta(t)} f(u, v).
\]
Problem 1.41 (Max-Flow). What is the maximum flow that can be established
between a source and a target node in a network?

Remarks:
• Max-Flow can be written as an LP maximizing the value of the flow.
• Flows are also useful to model discrete data. Imagine traffic flow for
example: every road as some capacity and at each intersection, every
car getting in is expected to eventually get out!
• Fortunately, we can use the linear relaxation of the ILP and be guaran-
teed to have the optimal solution!

Theorem 1.42 (Integral Flow Theorem). If the capacity of each edge is an
integer, then there exists a maximum flow such that every edge has an integral
flow.

Proof. Assume you have an optimal but non-integral flow. If there is a path
from s to t with every edge being non-integral, we can increase the flow on that
path, so our original flow was not optimal. Hence, there cannot be a non-integral
path from s to t.

Let \( u \) be a node adjacent to an edge \( e \) with non-integral flow. Then \( u \) needs
at least another edge \( e' \) with non-integral flow because of flow conservation at
node \( u \). We can follow these non-integral edges. Since they cannot include both
\( s \) and \( t \), we must find a cycle \( C \) of non-integral edges. All edges in \( C \) can both
change their flow by \( \pm \epsilon \), without changing the flow from \( s \) to \( t \). We change the
flow of all edges in \( C \) until a first edge in \( C \) has integral flow. Now we have one
edge less with non-integral flow. If there is still an edge with non-integral flow,
we repeat this procedure, until all edges have integral flow.

Remarks:
• Thanks to Theorem 1.42, we can solve a discrete maximum flow prob-
lem with the linear relaxation of the ILP formulation and the simplex
algorithm!
• There are also more efficient algorithms, known as augmenting paths
algorithms.

Definition 1.43 (Augmenting Path). We define an \textbf{augmenting path} as a
path from \( s \) to \( t \) such that the flow of each edge does not reach its capacity.

Algorithm 1.44: Find augmenting path

Remarks:
• If the network has an augmenting path, then none of the edge of this
path is at full capacity and we can add some flow on this path. This
gives us a greedy algorithm: Find an augmenting path, push as much
flow as possible on this path, then try again. This is known as the
Ford-Fulkerson algorithm.

Algorithm 1.45: Ford-Fulkerson algorithm

Chapter Notes
The word algorithm is derived from the name of Muhammad ibn Musa al-
Khwarizmi, a Persian mathematician who lived around AD 780–850. Some
algorithms are as old as civilizations. A division algorithm was already used by
the Babylonians around 2500 BCE. [2] Recursion Analyzing the time efficiency
of recursive algorithms is often a difficult task. An easy but powerful approach
is given by the master theorem [1]. Linear programming is an old concept whose
origins lie in solving logistic problems during World War 2. Back in the days,
the term programming meant optimization, and not coding. This chapter was written in collaboration with Henri Devillez and Roland Schmid.

Bibliography
