Chapter 5. Metaheuristics

Algorithmics and Programming III

FIB

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Chapter 5. Metaheuristics

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Computationally difficult problems

In this course we have mostly considered computationally intractable problems and ways to tackle them:

- For small inputs we can simply apply brute force
- For some problems, if enough memory is available we can apply dynamic programming
- For some problems, polynomial-time greedy algorithms can be used in certain subproblems
- Now we present metaheuristics: general strategies that guide the search to efficiently find (near-)optimal solutions

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- Now we present metaheuristics: general strategies that guide the search to efficiently find (near-)optimal solutions

Computationally difficult problems

We are interested in solving Combinatorial Optimization Problems (COP)

Formally, given

- a set of variables $X = (x_1, x_2, \ldots, x_n)$ with domains $D_1, D_2, \ldots, D_n$,
- a set of constraints $C_1, C_2, \ldots, C_m$ among variables (each constraint can be seen as a subset $C_i \subseteq D_1 \times D_2 \times \cdots D_n$),
- an objective function $f : D_1 \times D_2 \times \cdots D_n \rightarrow \mathbb{R}^+$,

we define the set of solutions $S := \cap_{i=1}^{m} C_i$.

Our goal is to find a (globally) optimal solution $s^* \in \underset{x \in S}{\text{argmin}}\ f(x)$.

EXAMPLES:

- Knapsack
- Min Graph Coloring
- Traveling Salesman Problem
- ...

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Chapter 5. Metaheuristics

Metaheuristics

- A metaheuristic is an algorithm for solving approximately a wide range of hard optimization problems without much adaptation to each problem
- Metaheuristics are:
  - efficient
  - approximate
  - non problem-specific
  - usually non-deterministic
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Metaheuristics

A key aspect of metaheuristics is to provide a balance between:

- Intensification:
  intensively explore areas of the search space with good solutions
- Diversification:
  move to unexplored areas of the search space when necessary

What determines the areas of the search space to explore is the concept of neighborhood:

- A neighborhood structure is a function $\mathcal{N} : S \to 2^S$.
  Given $s \in S$, we call $\mathcal{N}(s)$ the neighborhood of s.
- A local minimum wrt a neighborhood structure $\mathcal{N}$ is
  a solution $\hat{s}$ such that $\forall s \in \mathcal{N}(\hat{s}) : f(\hat{s}) \leq f(s)$

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Let us consider the Knapsack Problem:
given a set of items, each with a certain value and weight, the goal is to find a subset not exceeding a certain weight W and with maximum value

Item Id	1	2	3	4	5	6	7
Value	7	2	1	4	3	4	8
Weight	10	7	2	8	4	6	15

$W = 23$

Given a solution s, we could define $\mathcal{N}(s)$ as the set of solutions that:

- can be obtained from s by replacing one item by another one, and
- whose sum does not exceed W

For example:

- $\{7, 4\}$ belongs to $\mathcal{N}(\{7, 5\})$
- $\{7, 4\}$ is a local optimum
- However, it is not global. A global optimum is $\{1, 3, 5, 6\}$.

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Metaheuristics

Metaheuristics can be classified according to various criteria:

- Population-based vs single point search
- Dynamic vs static objective function
- One vs various neighborhood structures
- Memory usage vs memory-less methods
- Nature-inspired vs non-nature inspired

In the following we will introduce some of the most successful metaheuristics.
We will present them in their general setting,
without biasing them towards one concrete COP.

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Chapter 5. Metaheuristics

Basic Local Search: Iterative Improvement

Basic Local Search, a.k.a Iterative Improvement or Hill Climbing:

- Start with an arbitrary solution $s \in S$.
- While possible, replace s by an element of $\mathcal{N}(s)$ with smaller cost f

In Pseudo-code:

```
s := generateInitialSolution()
repeat
  s := Improve(N(s))
until no improvement is possible
```

The algorithm terminates at a local minimum,
but may not be a global minimum.

Basic Local Search: Iterative Improvement

This scheme indeed describes a large family of concrete algorithms:

- How do we choose the neighborhood structure $\mathcal{N}$?
  - It should be rich enough so that we do not tend to get stuck in bad local optima (see previous Knapsack example)
  - It should not be too large, since we want to be able to efficiently search the neighborhood for possible local moves
- How do we implement *Improve*$(\mathcal{N}(s))$?
  - **First improvement:** choose the first s' we find s.t. $f(s') < f(s)$
  - **Best improvement:** choose $s' \in \operatorname{argmin}_{\hat{s} \in \mathcal{N}(s)} f(\hat{s})$
    (i.e. explore the whole $\mathcal{N}(s)$ and pick the best element)

Iterative improvement disallows to temporarily worsen the objective function, and hence it cannot escape from bad local optima.

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Chapter 5. Metaheuristics

Simulated Annealing

- Fundamental idea: allow moves resulting in solutions of worse quality than the current solution in order to escape from local minima.
- The probability of doing such a move is decreased during the search

```
s := generateInitialSolution()
T := T0
while termination conditions not met do
    s' := pickAtRandom(N(s))
    if f(s') < f(s) then s' := s
    else with probability p(T,s',s), s' := s
    endif
    update(T)
endwhile
```

Simulated Annealing

- How is the probability of accepting a worsening move defined?
  - The probability is usually computed with the Boltzmann distribution

$$p(T, s', s) = exp(-\frac{f(s') - f(s)}{T})$$

  - Given a fixed temperature T, the closer $f(s')$ is to $f(s)$, the higher the probability of accepting the move
  - Given fixed s, s', since $f(s') > f(s)$, the higher the temperature T the higher the probability of accepting a worsening move
- How do we update the temperature?
  - The temperature at iteration k is defined as a function $Q(T_k, k)$ of the current temperature T_k and the iteration number
  - There are functions that guarantee the convergence to a global optimum, but they are too slow to be feasible in practice
  - One of the most useful functions follows a geometric law $T_{k+1} = \alpha \cdot T_k$, with $\alpha \in [0, 1]$.

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Chapter 5. Metaheuristics

Tabu Search

- The simplest form of Tabu Search applies a best-improvement local search as basic ingredient and uses a memory (tabu list) to escape from local minima and avoid cycles
- The tabu list keeps track of the most recently visited solutions. The solutions in the tabu list are excluded from the neighborhood of the current solution
- At each iteration, the best solution in neighborhood is chosen and added to the tabu list and the oldest of the solutions in the list is removed in a FIFO order.
- About the tabu-list length:
  - It controls the memory consumed by the process
  - With small lengths the search concentrates on small areas of the search space
  - With large lengths the search explores larger regions
  - The length can be varied dynamically during the search

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Tabu Search

- How do we store the solutions in the tabu list?
  - Storing complete solutions is impractical,
    and so only attributes are stored (e.g. components of solutions).
    One tabu list for each attribute is kept.
  - Forbidding an attribute assigns the tabu status to probably more than one solution. It is hence possible that unvisited solutions of good quality are excluded from the allowed set.
  - To overcome this problem, aspiration criteria are defined. They allow to move to a solution even if forbidden by the tabu conditions.

    Example: always allow moving to solutions that are better than the current best one.

Tabu Search

```
s := generateInitialSolution()
initializeTabuLists(TL_1, TL_2, ..., TL_r)
k := 0
while termination conditions not met do
    allowedSet = {s' ∈ N(s) | s' is not forbidden by tabu or
        satisfies some aspiration condition}
    s := chooseBestOf(allowedSet)
    updateTabuListAndAspirationConditions(s)
    k := k + 1
endwhile
```

Chapter 5. Metaheuristics

GRASP

- The Greedy Randomized Adaptive Search Procedure (GRASP) is a two-phase iterative procedure:
  - Phase 1: solution construction
  - Phase 2: solution improvement
- PHASE 1: Solution construction
  - Assume that a solution s consists of a subset of a set of elements (e.g. in knapsack it is a set of items).
    The solution is constructed by adding one new element at a time
  - Next element is chosen uniformly at random from a candidate list as follows
  - Each element is assigned a score that estimates the benefit if inserted into the current partial solution.
  - The Restricted Candidate List (RCL) is composed of the best α elements according to the scores.
  - For $\alpha = 1$ the construction amounts to a greedy heuristic.
    For $\alpha = n$, the construction is completely random.

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GRASP

- PHASE 1 in Pseudo-code:

```
s := ∅
α := determineCandidateListLength()
while solution not complete do
    RCL := generatedRestrictedCandidateList()
    x := selectElementAtRandom(RCL)
    s := s ∪ {x}
    updateGreedyFunction(s)
endwhile
```

- PHASE 2: Solution improvement
  - It is a local search process
    (Iterative Improvement, Simulated Annealing, Tabu Search, ...)
- The two phases are combined as follows:

```
while termination conditions not met do
    s := constructGreedyRandomizedSolution()
    s := applyLocalSearch(s)
    memorizeBestFoundSolution()
endwhile
```

GRASP

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GRASP

- GRASP is very effective if two conditions are satisfied:
  - Phase 1 samples the most promising regions of the search space
  - Phase 1 returns solutions belonging to basins of attraction of different local minima
- One drawback of GRASP is that it does not use the history of the search
- However, due to is simplicity, it is generally very fast and produces quite good solutions in a very short amount of time

Chapter 5. Metaheuristics

Variable Neighborhood Search

- Key idea of VNS: dynamically change neighborhood structures
- We assume a sequence of neighborhood structures $\mathcal{N}_1, \mathcal{N}_2, \ldots, \mathcal{N}_{kmax}$
- Although they could be arbitrary, usually $|\mathcal{N}_1| < |\mathcal{N}_2| < \ldots < |\mathcal{N}_{kmax}|$.
  As we will see, $\mathcal{N}_1 \subset \mathcal{N}_2 \subset \ldots \subset \mathcal{N}_{kmax}$ is not an efficient choice because work would be repeated.
- Starting with an initial solution s, the algorithm repeats three steps:
  1. Shaking: $s' \in \mathcal{N}_k(s)$ is randomly chosen
  2. Local search: obtain s'' from s' using any local search procedure
  3. Move:
     - if s'' better than s, replace it and set $k := 1$
     - otherwise $k := k + 1$

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Variable Neighborhood Search

Variable Neighborhood Search:

```
s := generateInitialSolution()
while termination conditions not met do
    k := 1
    while k < kmax do
        s' := pickAtRandom(N_k(s))
        s'' := localSearch(s')
        if f(s'') < f(s) then
            s := s''
            k := 1
        else
            k := k + 1
        endif
    endwhile
endwhile
```

Variable Neighborhood Search

- Shaking perturbs s to provide a good starting point for local search
- Ideally, s' should belong to the basin of attraction of another local minimum
- But it should not be too different from s. Otherwise, we are doing a simple random multi-start
- Intuitively, choosing s' in some neighborhood of s maintains some good features of s
- Changing neighborhood corresponds to a diversification of the search
- A solution that is locally optimal wrt one neighborhood is probably not locally optimal in another
- Different neighborhood structures have different landscape topologies, and hence search behave differently on them.
  This property is exploited by Variable Neighborhood Descent (VND)

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Variable Neighborhood Search

Variable Neighborhood Descent:

```
s := generateInitialSolution()
while termination conditions not met do
    k := 1
    while k < kmax do
        s' := chooseBestOf(N_k(s))
        if f(s') < f(s) then
            s := s'
            k := 1
        else
            k := k + 1
        endif
    endwhile
endwhile
```

- The choice of the neighborhoods is the critical point of VNS and VND.
- They should exploit different properties of the search space, i.e, should provide different abstractions of it.

Chapter 5. Metaheuristics

Guided Local Search

- In order to diversify the search and escape from local minima, GLS dynamically changes the objective function so as to make them less desirable.
- Let us fix a set of m solution features, which can be any kind of properties or characteristics that discriminate between solutions (e.g. in knapsack, a solution feature can be if a fixed object is chosen).
- We will use m indicator functions $I_i(s)$ that return value 1 iff the feature i is present in solution s.
- Each solution feature has a fixed associated cost c_i (e.g. in knapsack $-$value, the negated of the value).
- After every solution found, the new objective function f' is redefined by

$$f'(s) = f(s) + \lambda \sum_{i=1}^{m} p_i \cdot I_i(s)$$

where

  - λ is called the regularization parameter, and
  - p_i are the penalty parameters (which change during the execution)

Guided Local Search

- In Pseudo-code:

```
s := generateInitialSolution()
(p1,p2,...,pm) := (0,0,...,0)
while termination conditions not met do
    s := localSearch(s,f')
    update(p1,p2,...,pm)
endwhile
```

- Every time a local optimum is found, GLS tries to penalize the features of this solution with highest cost
- Given s, the utility of penalizing a feature i is

$$Util(s,i) = I_i(s) \cdot \frac{c_i}{1+p_i}$$

- When updating, for all features i such that $Util(s,i)$ is maximum, we set $p_i := p_i + 1$.
- This scheme penalizes features with highest cost c_i, but the presence of $1 + p_i$ dividing prevents a feature from being penalized again and again.

Chapter 5. Metaheuristics

Evolutionary Computation (Genetic Algorithms)

- At every iteration of the algorithm, we will deal with a set of solutions, to which we will refer as individuals.
- This population of individuals evolves at each iteration by the following rules:
  - New individuals are created by applying recombination, that combines two or more individuals (so-called parents) to produce one or more new individuals (children or offspring).
  - Mutation allows the appearance of new traits in the offspring to promote diversity.
  - Selection of which individuals will be maintained into the next generation is done by evaluating their fitness, i.e. how good they are.
- As a termination condition, a predefined number of generations may be used

Evolutionary Computation (Genetic Algorithms)

- In Pseudo-code:

```
P := generateInitialPopulation()
evaluate(P)
while termination conditions not met do
    Par := selectParents(P)
    P′ := recombine(Par)
    P″ := mutate(P′)
    evaluate(P″)
    P := select(P″ ∪ P)
endwhile
```

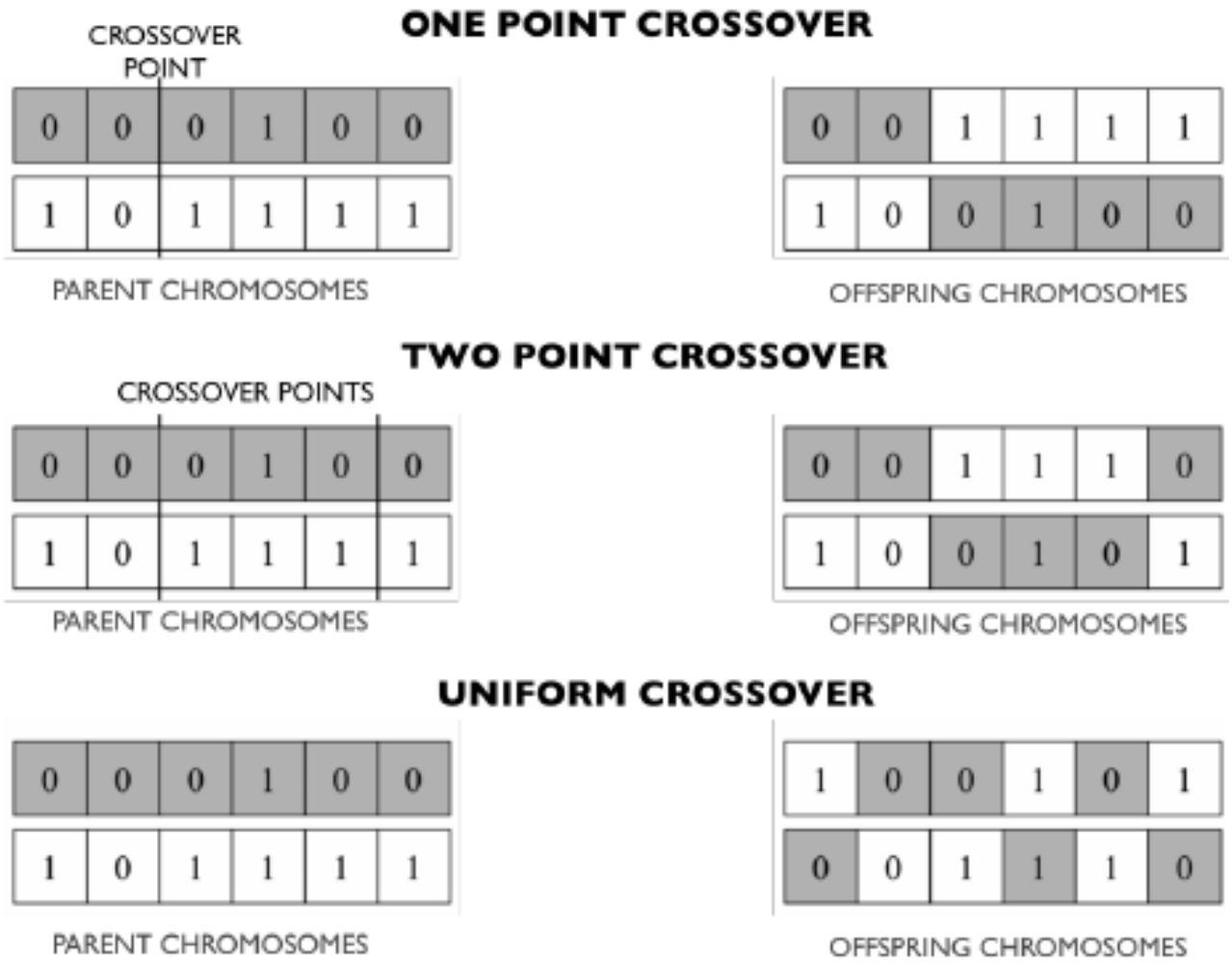
- A concrete instance is the well-known case of Genetic Algorithm

Genetic Algorithms:

- The basic GA is very generic. It will vary depending on: representation of individuals, selection strategy, recombination procedure and mutator operators.
- Representation of individuals: individuals are usually represented using bit-strings of fixed length, although permutations of integer numbers are also frequent
- Selection strategy for parents: after evaluating the fitness of each individual f_i, several selection strategies exist:
  - Roulette-wheel selection: the probability to choose one individual is $f_i / \sum_{j=1}^{n} f_j$
  - Ranking selection: sort all n individuals wrt their fitness. The i-th individual in order gets rank i. The probability to select an individual x is $2 \cdot rank(x)/(n \cdot (n-1))$.
  - Tournament selection: choose k elements at random and pick the one with the highest fitness. Repeat until selecting enough individuals to mate.

Evolutionary Computation (Genetic Algorithms)

- Recombination: it is called crossover in this context.
- When individuals are encoded as bit-strings, we can use, among others:



- Recombination: it is called crossover in this context.
- When individuals are encoded permutations of integers, we can use, among others:
  - Partially-mapped crossover:

$P_1 = (1\ 2\ 3 \mid 4\ 5\ 6\ 7 \mid 8\ 9)$ `Select two random cut points`
$P_2 = (4\ 5\ 2 \mid 1\ 8\ 7\ 6 \mid 9\ 3)$

$O_1 = (\quad\quad \mid 1\ 8\ 7\ 6 \mid \quad\quad)$
$O_2 = (\quad\quad \mid 4\ 5\ 6\ 7 \mid \quad\quad)$

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$P_2 = (4\ 5\ 2 \mid 1\ 8\ 7\ 6 \mid 9\ 3)$

$O_1 = (\quad\quad \mid 1\ 8\ 7\ 6 \mid \quad\quad)$
$O_2 = (\quad\quad \mid 4\ 5\ 6\ 7 \mid \quad\quad)$

This induces mappings

$$\sigma(1) = 4, \tau(4) = 1$$
$$\sigma(8) = 5, \tau(5) = 8$$
$$\sigma(7) = 6, \tau(6) = 7$$

We can fill the leftmost and the rightmost parts O_1 as P_1.
If there is a conflict, use mapping σ.

Similarly with O_2 using mapping τ.

Evolutionary Computation (Genetic Algorithms)

- Recombination: it is called crossover in this context.
- When individuals are encoded permutations of integers, we can use, among others:
  - Partially-mapped crossover:

    $P_1 = (1\ 2\ 3 \mid 4\ 5\ 6\ 7 \mid 8\ 9)$ `Select two random cut points`
    $P_2 = (4\ 5\ 2 \mid 1\ 8\ 7\ 6 \mid 9\ 3)$

    $O_1 = (4\ 2\ 3 \mid 1\ 8\ 7\ 6 \mid 5\ 9)$
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    This induces mappings
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To generate O_2, take its order 9 3 4 5 2 1 8 7 6 and remove $\{4, 5, 6, 7\}$. We obtain the order 9 3 2 1 8, that we use to fill it

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Evolutionary Computation (Genetic Algorithms)

- Mutator operators:
  - Introduces some randomness to prevent the optimization from getting trapped in local optima
  - Typically, mutation is applied with less than 1% probability
  - Examples:
    - For bit-strings: randomly flip the value of one bit
    - For permutations of integers: swap two numbers, remove one number (or a sequence of them) and insert in somewhere else, etc.
  - Selection of new generation individuals:
    - We use again the fitness function to evaluate the quality of individuals
    - Usually, one keeps the best individuals from the previous generation
    - Among the offsprings, a subset of them is selected according to their fitness
    - One can decide to keep a fixed-size population or vary its size

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Chapter 5. Metaheuristics

Swarm Intelligence (Ant Colony Optimization)

- Swarm Intelligence is a paradigm for solving optimization problems inspired by the collective behavior of social insect colonies or animal societies.
- SI systems are made up of a population of simple agents interacting locally with one another and the environment
- These entities with very limited individual capability can jointly perform complex tasks necessary for their survival
- Although there is normally no centralized control structure, local interactions between agents often lead to global and self-organized behavior.
- Examples:
  - Ant Colony Optimization
  - Particle Swarm Intelligence
  - Bacterial Foraging Optimization
  - Bee Colony Optimization
  - ...

Swarm Intelligence (Ant Colony Optimization)

- We will focus on Ant Colony Optimization (ACO)
- ACO takes inspiration from the foraging behavior of real ants:
  - When searching for food, ants initially explore the area surrounding their nest with randomized walk
  - While walking, ants deposit a chemical pheromone trail on the ground to mark some favorable path that should guide other ants to the food source
  - After some time, the shortest path to the food source contains a higher concentration of pheromone and, therefore, attracts more ants

Swarm Intelligence (Ant Colony Optimization)

- ACO creates a set of m ants, which are in charge of incrementally and stochastically building solutions starting from the empty solution $s_p = \emptyset$. Intermediate solutions are referred to as solution states.
- At each step, each ant moves from a state x to state y, corresponding to adding a new element to the solution.
- How do we decide which transition is chosen?
  - The next state can only be chosen from the set of valid transitions $\mathcal{V}(x) = \{y \mid y \text{ if feasible and } x \to y \text{ is a transition}\}$.
  - Each valid transition has associated a dynamic value $\tau_{x,y}$ (pheromone) and fixed value $\eta_{i,j}$ (heuristic information about the problem)
  - The probability of choosing $x \to y$ is:

$$Prob(x \to y) = \frac{\tau_{x,y}^{\alpha} \cdot \eta_{x,y}^{\beta}}{\sum_{z \in \mathcal{V}(x)} \tau_{x,z}^{\alpha} \cdot \eta_{x,z}^{\beta}}$$

    with constants $\alpha, \beta \geq 0$

- How are the pheromone values $\tau_{x,y}$ updated to bias the ants towards good solutions?
  - We want to achieve two goals:
    - Move ants towards high-quality states. Pheromone values for good transitions should be increased (intensification)
    - Avoid ants from always going to the same state. Pheromone values should be evaporated (diversification)
  - Initially we can assume that all $\tau_{x,y}$ are equal
  - Once every ant has constructed a solution, we select of set S_{hq} of high-quality solutions. We update the pheromones $\tau_{x,y}$ as follows:

$$\tau_{x,y} := (1-\rho)\tau_{x,y} \quad + \sum_{s \in S_{hq} | y-x \subseteq s} f(s)$$

where $\rho \in (0,1]$ is the evaporation rate and $f(s)$ is the fitness function ($f : S \to \mathbb{R}^+$ such that $F(s) < F(s') \implies f(s) \geq f(s')$, where F is the function to minimize)

Swarm Intelligence (Ant Colony Optimization)

The overall ACO algorithm is:

```
Initialize pheromone values
while termination conditions not met do
    Construct Ants Solutions
    Update Pheromones
    Daemon Actions
endwhile
```

Daemon Actions refer to any centralized operation that a single ant cannot perform. The most used one is the application of local search to the constructed solutions.