Ant Colony Optimization

Part 4: Implementing ACO Algorithms

Spring 2009
Instructor: Dr. Masoud Yaghini
Ant Colony Optimization: Part 4

Outline

- Data Structures
- The Algorithm
- Changes for Other ACO Algorithms
- References
Data Structures
Data Structures

- We mainly focus on **AS** and indicate, where appropriate, the necessary changes for implementing other ACO algorithms.

- **Data Structures**
  - Problem Representation
    - Intercity Distances
    - Nearest-Neighbor Lists
    - Pheromone Trails
    - Combining Pheromone and Heuristic Information
  - Representing Ants
    - Ant’s Memory Storing (partial) Tours
    - Visited Cities
Main data structures

% Representation of problem data

integer dist[n][n]  % distance matrix
integer nn_list[n][nn]  % matrix with nearest neighbor lists of depth nn
real pheromone[n][n]  % pheromone matrix
real choice_info[n][n]  % combined pheromone and heuristic information

% Representation of ants

structure single_ant
begin
  integer tour_length % the ant’s tour length
  integer tour[n + 1] % ant’s memory storing (partial) tours
  integer visited[n] % visited cities
end

single_ant ant[m]  % structure of type single_ant
Intercity Distances

- Often a symmetric TSP instance is given as the coordinates of a number of $n$ points.
- In this case, one possibility would be to store the $x$ and $y$ coordinates of the cities in two arrays and then compute on the fly the distance between the cities as needed. However, this leads to a significant computational overhead.
- It is more reasonable to precompute all intercity distances and to store them in a symmetric distance matrix with $n^2$ entries, integer $dist[n][n]$. 

For symmetric TSPs we only need to store $\frac{n(n-1)}{2}$ distinct distances,

It is more efficient to use an $n^2$ matrix to avoid performing additional operations to check whether, when accessing a generic distance $d(i, j)$, entry $(i, j)$ or entry$(j, i)$ of the matrix should be used.
It is also important to know that, for historical reasons, in almost all the TSP literature, the distances are stored as integers.

In fact, in old computers integer operations used to be much faster than operations on real numbers, so that by setting distances to be integers, much more efficient code could be obtained.
Nearest-Neighbor Lists

- In addition to the distance matrix, it is convenient to store for each city a list of its nearest neighbors.
- Let $d_i$ be the list of the distances from a city $i$ to all cities $j$, with $j = 1, \ldots, n$ and $i \neq j$
- The nearest-neighbor list of a city $i$ is obtained by sorting the list $d_i$ according to nondecreasing distances, obtaining a sorted list $d'_i$, ties can be broken randomly.
Nearest-Neighbor Lists

- The position $r$ of a city $j$ in city $i$’s nearest-neighbor list $nn_list[i]$ is the index of the distance $d_{ij}$ in the sorted list $d'_i$

- $nn_list[i][r]$ gives the identifier (index) of the $r$-th nearest city to city $i$
  - i.e., $nn_list[i][r] = j$

- You have to repeat a sorting algorithm over $n - 1$ cities for each city
Nearest-Neighbor Lists

- An enormous speedup is obtained for the solution construction in ACO algorithms.
- If the nearest-neighbor list is cut $nn$ after a constant number $nn$ of nearest neighbors, where typically $nn$ is a small value ranging between 15 and 40.
- In this case, an ant located in city $i$ chooses the next city among the $nn$ nearest neighbors of $i$.
- In case the ant has already visited all the nearest neighbors, then it makes its selection among the remaining cities.
It should be noted that the use of truncated nearest-neighbor lists can make it impossible to find the optimal solution.
Pheromone Trails

- In addition to the instance-related information, we also have to store for each connection \((i, j)\) a number \(\tau_{ij}\) corresponding to the pheromone trail associated with that connection.
- For symmetric TSPs this requires storing \(n(n-1)/2\) distinct pheromone values, because we assume that \(\tau_{ij} = \tau_{ji}\), for all \((i, j)\)
- Again, as was the case for the distance matrix, it is more convenient to use some redundancy and to store the pheromones in a symmetric \(n^2\) matrix.
When constructing a tour, an ant located on city $i$ chooses the next city $j$ with a probability which is proportional to the value of $[\tau_{ij}]^\alpha[\eta_{ij}]^\beta$.

Because these very same values need to be computed by each of the $m$ ants, computation times may be significantly reduced by using an additional matrix $\text{choice} \_\text{info}[n][n]$.

Each entry $\text{choice} \_\text{info}[i][j]$ stores the value $[\tau_{ij}]^\alpha[\eta_{ij}]^\beta$. 
Combining Pheromone and Heuristic Information

- Again, in the case of a symmetric TSP instance, only $n(n-1)/2$ values have to be computed, but it is convenient to store these values in a redundant way as in the case of the pheromone and the distance matrices.

- Additionally, one may store the $[\eta_{ij}]^\beta$ values in a further matrix heuristic to avoid recomputing these values after each iteration, because the heuristic information stays the same throughout the whole run of the algorithm.
Finally, if some distances are zero, which is in fact the case for some of the benchmark instances in the TSPLIB, then one may set them to a very small positive value to avoid division by zero.
Representing Ants

- An ant is a simple computational agent which
  - constructs a solution to the problem at hand, and
  - may deposit an amount of pheromone $\Delta \tau$ on the arcs it has traversed.

- To do so, an ant must be able to
  - (1) store the partial solution it has constructed so far,
  - (2) determine the feasible neighborhood at each city, and
  - (3) compute and store the objective function value of the solutions it generates.
Ant’s memory storing (partial) tours

- The first requirement can be satisfied by storing the partial tour in a sufficiently large array.
- For the TSP we represent tours by arrays of length $n + 1$, integer $\text{tour}[n + 1]$, where at position $n + 1$ the first city is repeated.
- This choice makes easier some of the other procedures like the computation of the tour length.
Visited Cities

- The knowledge of the partial tour at each step is sufficient to allow the ant to determine whether a city j is in its feasible neighborhood:
  - it is enough to scan the partial tour for the occurrence of city j.
  - If city j has not been visited yet, then it is member of the feasible neighborhood; otherwise it is not.

- Unfortunately, this simple way of determining the feasible neighborhood involves a high computational overhead.
Visited Cities

- The simplest way around this problem is to associate with each ant an additional array visited whose values are set to $\text{visited}[j] = 1$ if city $j$ has already been visited by the ant, and to $\text{visited}[j] = 0$ otherwise.

- This array is updated by the ant while it builds a solution.

- The array visited, part of the data structure `single_ant`, is declared of type `integer`; however, to save memory, it could be declared of type `Boolean`
Tour Length

- Finally, the computation of the tour length, stored by the ant in the `tour_length` variable, can be done by summing the length of the $n$ arcs in the ant’s tour.
Overall Memory Requirement

- For representing all the necessary data for the problem we need:
  - four matrices of dimension \( n \times n \) for representing the distance matrix, the pheromone matrix, the heuristic information matrix, and the choice_info matrix, and
  - a matrix of size \( n \times nn \) for the nearest-neighbor lists.
  - two arrays of size \( (n +1) \) and \( n \) to store the tour and the visited cities
  - an integer for storing the tour’s length.
  - a variable for representing each of the \( m \) ants
  - the best solution found so far
  - statistical information about the algorithm performance
The Algorithm
The main tasks to be considered in an ACO algorithm are:
  - the solution construction,
  - the management of the pheromone trails, and
  - the additional techniques such as local search.

In addition, the data structures and parameters need to be initialized and some statistics about the run need to be maintained.

In this section we give some details on how to implement the different procedures of AS in an efficient way.
The Algorithm

- A high-level view of the algorithm:

```plaintext
procedure ACOforTSP
    InitializeData
    while (not terminate) do
        ConstructSolutions
        LocalSearch
        UpdateStatistics
        UpdatePheromoneTrails
    end-while
end-procedure
```
Data Initialization

- **Data initialization:**
  - (1) the instance has to be read;
  - (2) the distance matrix has to be computed;
  - (3) the nearest-neighbor lists for all cities have to be computed;
  - (4) the pheromone matrix and the choice_info matrix have to be initialized;
  - (5) the ants have to be initialized;
  - (6) the algorithm’s parameters must be initialized; and
  - (7) some variables that keep track of statistical information, such as the used CPU time, the number of iterations, or the best solution found so far, have to be initialized.
Data Initialization

- A possible organization of these tasks into several data initialization procedures is indicated in the figure:

```plaintext
procedure InitializeData
    ReadInstance
    ComputeDistances
    ComputeNearestNeighborLists
    ComputeChoiceInformation
    InitializeAnts
    InitializeParameters
    InitializeStatistics
end-procedure
```
Termination Condition

- The program stops if at least one termination condition applies. Possible termination conditions are:
  - (1) the algorithm has found a solution within a predefined distance from a lower bound on the optimal solution quality;
  - (2) a maximum number of tour constructions or a maximum number of algorithm iterations has been reached;
  - (3) a maximum CPU time has been spent; or
  - (4) the algorithm shows stagnation behavior.
The solution construction requires the following phases.

1. First, the ants’ memory must be emptied.
   - This is done in lines 1 to 5 of procedure ConstructSolutions by marking all cities as unvisited, that is, by setting all the entries of the array ants.visited to false for all the ants.

2. Second, each ant has to be assigned an initial city.
   - One possibility is to assign each ant a random initial city.
   - This is accomplished in lines 6 to 11 of the procedure.
   - The function random returns a random number chosen according to a uniform distribution over the set \{1,…,n\}. 
3. Next, each ant constructs a complete tour.
   – At each construction step the ants apply the AS action choice rule [equation (3.2)].
   – The procedure `ASDecisionRule` implements the action choice rule and takes as parameters the ant identifier and the current construction step index; this is discussed later in more detail.

4. Finally, the ants move back to the initial city and the tour length of each ant’s tour is computed.
   – This is done in lines 18 to 21.
   – for the sake of simplicity, in the tour representation we repeat the identifier of the first city at position $n + 1$; this is done in line 19.
Solution Construction

procedure ConstructSolutions
1   for $k = 1$ to $m$ do
2       for $i = 1$ to $n$ do
3           ant[$k$].visited[$i$] ← false
4       end-for
5   end-for
6   step ← 1
7   for $k = 1$ to $m$ do
8       $r ← \text{random}\{1,\ldots,n\}$
9       ant[$k$].tour[step] ← $r$
10      ant[$k$].visited[$r$] ← true
11   end-for
Solution Construction

12 \textbf{while} (step < n) \textbf{do} \\
13 \hspace{1em} step \leftarrow step + 1 \\
14 \hspace{1em} \textbf{for} k = 1 \textbf{ to } m \textbf{ do} \\
15 \hspace{2em} \text{ASDecisionRule}(k, \text{step}) \\
16 \hspace{1em} \textbf{end-for} \\
17 \textbf{end-while} \\
18 \textbf{for} k = 1 \textbf{ to } m \textbf{ do} \\
19 \hspace{1em} \text{ant}[k].\text{tour}[n + 1] \leftarrow \text{ant}[k].\text{tour}[1] \\
20 \hspace{1em} \text{ant}[k].\text{tour\_length} \leftarrow \text{ComputeTourLength}(k) \\
21 \hspace{1em} \textbf{end-for} \\
\textbf{end-procedure}
Solution Construction

- As stated above, the solution construction of all of the ants is synchronized in such a way that the ants build solutions in parallel.

- The same behavior can be obtained, for all AS variants, by ants that construct solutions sequentially, because the ants do not change the pheromone trails at construction time.

- This is not the case for ACS, in which case the sequential and parallel implementations give different results.
In the action choice rule an ant located at city i probabilistically chooses to move to an unvisited city j based on the pheromone trails $[\tau_{ij}]^\alpha$ and the heuristic information $[\eta_{ij}]^\beta$ by see equation:

$$p_{ij}^k = \frac{[\tau_{ij}]^\alpha[\eta_{ij}]^\beta}{\sum_{l \in \mathcal{N}_i^k} [\tau_{il}]^\alpha[\eta_{il}]^\beta}, \quad \text{if } j \in \mathcal{N}_i^k$$
ASDecisionRule Procedure

- AS without candidate lists: pseudo-code for the action choice rule.

```plaintext
procedure ASDecisionRule(k, i)
  input k  % ant identifier
  input i  % counter for construction step
  c ← ant[k].tour[i − 1]
  sum_probabilities = 0.0
  for j = 1 to n do
    if ant[k].visited[j] then
      selection_probability[j] ← 0.0
    else
      selection_probability[j] ← choice_info[c][j]
      sum_probabilities ← sum_probabilities + selection_probability[j]
    end-if
  end-for
```
ASDecisionRule Procedure

11 \( r \leftarrow \text{random}[0, \text{sum}_\text{probabilities}] \)
12 \( j \leftarrow 1 \)
13 \( p \leftarrow \text{selection}_\text{probability}[j] \)
14 \hspace{1em} \text{while} (p < r) \text{ do} \)
15 \hspace{2em} j \leftarrow j + 1 \)
16 \hspace{2em} p \leftarrow p + \text{selection}_\text{probability}[j] \)
17 \hspace{1em} \text{end-while} \)
18 \hspace{1em} \text{ant}[k].\text{tour}[i] \leftarrow j \)
19 \hspace{1em} \text{ant}[k].\text{visited}[j] \leftarrow \text{true} \)

end-procedure
The procedure works as follows:

1. First, the current city \( c \) of ant \( k \) is determined (line 1).

2. The probabilistic choice of the next city then works analogously to the roulette wheel selection procedure of evolutionary computation:
   - each value \( \text{choice}_i[c][j] \) of a city \( j \) that ant \( k \) has not visited yet determines a slice on a circular roulette wheel, the size of the slice being proportional to the weight of the associated choice (lines 2–10).
Solution Construction

- 3. the wheel is spun and the city to which the marker points is chosen as the next city for ant $k$ (lines 11–17).

- This is implemented by:
  - summing the weight of the various choices in the variable `sum_probabilities`,
  - drawing a uniformly distributed random number $r$ from the interval $[0, \text{sum\_probabilities}]$,
  - going through the feasible choices until the sum is greater or equal to $r$. 
4. Finally, the ant is moved to the chosen city, which is marked as visited (lines 18 and 19).
Solution Construction

- When exploiting candidate lists, the procedure \texttt{ASDecisionRule} needs to be adapted, resulting in the procedure \texttt{NeighborListASDecisionRule}.
- A first change is that when choosing the next city, one needs to identify the appropriate city index from the candidate list of the current city $c$.
- This results in changes of the maximum value of index $j$ is changed from $n$ to $nn$ in line 3 and the test performed in line 4 is applied to the $j$-th nearest neighbor given by $nn\_list[c][j]$. 
A second change is necessary to deal with the situation in which all the cities in the candidate list have already been visited by ant $k$.

In this case, the variable `sum_probabilities` keeps its initial value 0.0 and one city out of those not in the candidate list is chosen.

The procedure `ChooseBestNext` is used to identify the city with maximum value of $[\tau_{ij}]^\alpha[\eta_{ij}]^\beta$ as the next to move to.
Solution Construction

- AS with candidate lists: pseudo-code for the action choice rule.

```plaintext
procedure NeighborListASDecisionRule(k, i)
    input k % ant identifier
    input i % counter for construction step

    c ← ant[k].tour[i - 1]
    sum_probabilities ← 0.0

    for j = 1 to nn do
        if ant[k].visited[nn_list[c][j]] then
            selection_probability[j] ← 0.0
        else
            selection_probability[j] ← choice_info[c][nn_list[c][j]]
            sum_probabilities ← sum_probabilities + selection_probability[j]
        end-if
    end-for
```
Ant Colony Optimization: Part 4

Solution Construction

```
11 if (sum_probabilities = 0.0) then
12     ChooseBestNext(k, i)
13 else
14     r ← random[0, sum_probabilities]
15     j ← 1
16     p ← selection_probability[j]
17     while (p < r) do
18         j ← j + 1
19         p ← p + selection_probability[j]
20     end-while
21     ant[k].tour[i] ← nn_list[c][j]
22     ant[k].visited[nn_list[c][j]] ← true
23 end-if
end-procedure
```
Ant Colony Optimization: Part 4

Solution Construction

procedure ChooseBestNext(k, i)
    input k % ant identifier
    input i % counter for construction step
    v ← 0.0
    c ← ant[k].tour[i − 1]
    for j = 1 to n do
        if not ant[k].visited[j] then
            if choice_info[c][j] > v then
                nc ← j % city with maximal ταηβ
                v ← choice_info[c][j]
            end-if
        end-if
    end-for
    ant[k].tour[i] ← nc
    ant[k].visited[nc] ← true
end-procedure
Local Search

- Once the solutions are constructed, they may be improved by a local search procedure.
- While a simple 2-opt local search can be implemented in a few lines, the implementation of an efficient variant is somewhat more involved.
- Since the details of the local search are not important for understanding how ACO algorithms can be coded efficiently, we refer to the accompanying code (available at www.aco-metaheuristic.org/aco-code/) for more information on the local search implementation.
The last step in an iteration of AS is the pheromone update.

This is implemented by the procedure ASPheromoneUpdate, which comprises two pheromone update procedures: pheromone evaporation and pheromone deposit.

The first one, Evaporate decreases the value of the pheromone trails on all the arcs (i, j) by a constant factor r.
Pheromone Update

- The second one, DepositPheromone, adds pheromone to the arcs belonging to the tours constructed by the ants.

- Additionally, the procedure ComputeChoiceInformation computes the matrix choice_info to be used in the next algorithm iteration.

- Note that in both procedures care is taken to guarantee that the pheromone trail matrix is kept symmetric, because of the symmetric TSP instances.
Ant Colony Optimization: Part 4

Pheromone Update

- **AS**: management of the pheromone updates.

```
procedure ASPheromoneUpdate
    Evaporate
    for \( k = 1 \) to \( m \) do
        DepositPheromone(\( k \))
    end-for
    ComputeChoiceInformation
end-procedure
```
Ant Colony Optimization: Part 4

Pheromone Update

- AS: implementation of the pheromone evaporation procedure.

```plaintext
procedure Evaporate
    for i = 1 to n do
        for j = i to n do
            pheromone[i][j] ← (1 - ρ) · pheromone[i][j]
        end-for
        pheromone[j][i] ← pheromone[i][j]  % pheromones are symmetric
    end-for
end-procedure
```
Pheromone Update

- **AS**: implementation of the pheromone deposit procedure.

```plaintext
procedure DepositPheromone(k)
    input k  % ant identifier
    \( \Delta \tau \leftarrow 1/ant[k].tour\_length \)
    for \( i = 1 \) to \( n \) do
        \( j \leftarrow ant[k].tour[i] \)
        \( l \leftarrow ant[k].tour[i + 1] \)
        \( \text{pheromone}[j][l] \leftarrow \text{pheromone}[j][l] + \Delta \tau \)
        \( \text{pheromone}[l][j] \leftarrow \text{pheromone}[j][l] \)
    end-for
end-procedure
```
When attacking large TSP instances, profiling the code showed that the pheromone evaporation and the computation of the choice_info matrix for AS can require a considerable amount of computation time.

But in ACS only the pheromone trails of arcs that are crossed by some ant have to be changed and the number of ants in each iteration is a low constant.
Ant Colony Optimization: Part 4

Statistical Information

- The last step in the implementation of AS is to store statistical data on algorithm behavior such as:
  - the best-found solution since the start of the algorithm run,
  - the iteration number at which the best solution was found

- Details about these procedures are available at www.aco-metaheuristic.org/aco-code/.
Changes for Other ACO Algorithms
Changes for Other ACO Algorithms

- Some of the necessary adaptations are described when implementing AS variants, in the following:

1. When depositing pheromone, the solution may be given some weight, as is the case in EAS and AS_{rank}. This can be accomplished by simply adding a weight factor as an additional argument of the procedure DepositPheromone.

2. MMAS has to keep track of the pheromone trail limits. The best way to do so is to integrate this into the procedure ASPheromoneUpdate.
3. Finally, the search control of some of the AS variants may need minor changes. Examples are occasional pheromone trail **reinitializations** or the schedule for the frequency of the best-so-far update in MMAS.
Changes for Other ACO Algorithms

- Unlike AS variants, the implementation of ACS requires more significant changes, as listed in the following:

- 1. The implementation of the pseudorandom proportional action choice rule requires the generation of a random number $q$ uniformly distributed in the interval $[0, 1]$ and the application of the procedure `ChooseBestNext` if $q < q_0$, or of the procedure `ASDecisionRule` otherwise.
2. The local pheromone update can be managed by the procedure `ACSLocalPheromoneUpdate` (see the figure) that is always invoked immediately after an ant moves to a new city.

3. The implementation of the global pheromone trail update is similar to the procedure for the local pheromone update except that pheromone trails are modified only on arcs belonging to the best-so-far tour.
Changes for Other ACO Algorithms

- Implementation of the local pheromone update in ACS.

```plaintext
procedure ACSLocalPheromoneUpdate(k, i)
    input k % ant identifier
    input i % counter for construction step
    h ← ant[k].tour[i - 1]
    j ← ant[k].tour[i]
    pheromone[h][j] ← (1 - ξ)pheromone[h][j] + ξτ₀
    pheromone[j][h] ← pheromone[h][j]
    choice_info[h][j] ← pheromone[h][j] · exp(1/dist[h][j], β)
    choice_info[j][h] ← choice_info[h][j]
end-procedure
```
Ant Colony Optimization: Part 4

Changes for Other ACO Algorithms

4. The integration of the computation of new values for the matrix `choice_info` into the local and the global pheromone trail update procedures.
References
References

The End