# DM872 <br> Mathematical Optimization at Work 

## TSP practice

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## Outline

# 1. Dynamic Programming 

2. MILP Formulations
3. Solving the DFJ Formulation

## Traveling Salesman Problem

https://www.math.uwaterloo.ca/tsp/

## Outline

## 1. Dynamic Programming

## 2. MILP Formulations

## 3. Solving the DFJ Formulation

## Dynamic Programming

- Dynamic Programming (DP) is a technique to solve combinatorial optimization problems with applications, for example, in mathematical programming, optimal control, and economics
- DP is somehow related to branch-and-bound as it performs an intelligent enumeration of the feasible solutions of the problem considered
- Principle of Optimality (known as Bellman Optimality Conditions): Suppose that the solution of a problem is the result of a sequence of $n$ decisions $D_{1}, D_{2}, \ldots, D_{n}$; if a given sequence is optimal, then the first k decisions must be optimal, but also the last $n-k$ decisions must be optimal
- DP breaks down the problem into stages, at which decisions take place, and find a recurrence relation that relates each stage with the previous one


## Principle of Optimality

The TSP asks for the shortest tour that starts from 0 , visits all cities of the set $C=\{1,2, \ldots, n\}$ exactly once, and returns to 0 , where the cost to travel from $i$ to $j$ is $c_{i j}$ (with $(i, j) \in A$ ) If the optimal solution of a TSP with six cities is ( $0,1,3,2,4,6,5,0$ ), then...

- the optimal solution to visit $\{1,2,3,4,5,6\}$ starting from 0 and ending at 5 is $(0,1,3,2,4,6,5)$
- the optimal solution to visit $\{1,2,3,4,6\}$ starting from 0 and ending at 6 is ( $0,1,3,2,4,6$ )
- the optimal solution to visit $\{1,2,3,4\}$ starting from 0 and ending at 4 is $(0,1,3,2,4)$
- the optimal solution to visit $\{1,2,3\}$ starting from 0 and ending at 2 is $(0,1,3,2)$
- the optimal solution to visit $\{1,3\}$ starting from 0 and ending at 3 is $(0,1,3)$
- the optimal solution to visit 1 starting from 0 is $(0,1)$
$\rightsquigarrow$ The optimal solution is made up of a number of optimal solutions of smaller subproblems


## Enumerate All Solutions of the TSP

- A solution of a TSP with $n$ cities derives from a sequence of $n$ decisions, where the $k$ th decision consists of choosing the $k$ th city to visit in the tour

- The number of nodes (or states) grows exponentially with $n$
- At stage $k$, the number of states is $\binom{n}{k} k$ !
- With $n=6$, at stage $k=6,720$ states are necessary
$\rightsquigarrow$ DP finds the optimal solution by implicitly enumerating all states but actually generating only some of them


## Are All States Necessary?



If path $(0,1,2,3)$ costs less than $(0,2,1,3)$, the optimal solution cannot be found in the blue part of the tree

## Are All States Necessary?



If path $(0,1,2,3,4,5)$ costs less than $(0,1,2,4,3,5)$, the optimal solution cannot be found in the blue part of the tree

## Are All States Necessary?

- At stage $k(1 \leq k \leq n)$, for each subset of cities $S \subseteq C$ of cardinality $k$, it is necessary to have only $k$ states (one for each of the cities of the set $S$ )
- At state $k=3$, given the subset of cities $S=\{1,2,3\}$, three states are needed:
- the shortest-path to visit $S$ by starting from 0 and ending at 1
- the shortest-path to visit $S$ by starting from 0 and ending at 2
- the shortest-path to visit $S$ by starting from 0 and ending at 3
- At stage $k,\binom{n}{k} k$ states are required to compute the optimal solution (not $\binom{n}{k} k!$ )

| \#States $\mathrm{n}=6$ |  |  |
| :---: | :---: | :---: |
| Stage | $\binom{n}{k} k$ ! | $\binom{n}{k} k$ |
| 1 | 6 | 6 |
| 2 | 30 | 30 |
| 3 | 120 | 60 |
| 4 | 360 | 60 |
| 5 | 720 | 30 |
| 6 | 720 | 6 |

## Complete Trees with $\mathrm{n}=4$

Enumeration of all paths


Implicit enumeration of all paths


## Dynamic Programming Recursion for the TSP I

- Given a subset $S \subseteq C$ of cities and $k \in S$, let $f(S, k)$ be the optimal cost of starting from 0 , visiting all cities in $S$, and ending at $k$
- Begin by finding $f(S, k)$ for $|S|=1$, which is $f(\{k\}, k)=c_{0 k}, \forall k \in C$
- To compute $f(S, k)$ for $|S|>1$, the best way to visit all cities of $S$ by starting from 0 and ending at $k$ is to consider all $j \in S \backslash\{k\}$ immediately before $k$, and look up $f(S \backslash\{k\}, j)$, namely

$$
f(S, k)=\min _{j \in S \backslash\{k\}}\left\{f(S \backslash\{k\}, j)+c_{j k}\right\}
$$



- The optimal solution cost $z^{*}$ of the TSP is $z^{*}=\min _{k \in C}\left\{f(C, k)+c_{k 0}\right\}$


## Dynamic Programming Recursion for the TSP II

DP Recursion from [Held and Karp (1962)]

1. Initialization. Set $f(\{k\}, k)=c_{0 k}$ for each $k \in C$
2. RecursiveStep. For each stage $r=2,3, \ldots, n$, compute

$$
f(S, k)=\min _{j \in S \backslash\{k\}}\left\{f(S \backslash\{k\}, j)+c_{j k}\right\} \forall S \subseteq C:|S|=r \text { and } \forall k \in S
$$

3. Optimal Solution. Find the optimal solution cost $z^{*}$ as

$$
z^{*}=\min _{k \in C}\left\{f(C, k)+c_{k 0}\right\}
$$

- With the DP recursion, TSP instances with up to 25-30 customers can be solved to optimality; other solution techniques (i.e., branch-and-cut) are able to solve TSP instances with up to... 85900 customers
- Nonetheless, DP recursions represents the state-of-the-art solution techniques to solve a wide variety of PDPs


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3. Solving the DFJ Formulation

## 

- Find the cheapest movement for a drilling, welding, drawing, soldering arm as, for example, in a printed circuit board manufacturing process or car manufacturing process
- $n$ locations, asymmetric $c_{i j}$ cost of travel,


## Variables:

$$
x_{i j} \in\{0,1\} \quad \forall i, j \in V, i \neq j
$$

## Objective:

$$
\sum_{i=1}^{n} \sum_{j=1}^{n} c_{i j} x_{i j}
$$

## Constraints:

- visit all vertices

$$
\begin{array}{ll}
\sum_{j: j \neq i} x_{i j}=1 & \forall i=1, \ldots, n \\
\sum_{i: i \neq j} x_{i j}=1 & \forall j=1, \ldots, n
\end{array}
$$

- cut set constraints

$$
\sum_{i \in S} \sum_{j \notin S} x_{i j} \geq 1
$$

$$
\forall S \subset N, S \neq \emptyset
$$

- subtour elimination constraints

$$
\sum_{i \in S} \sum_{j \in S} x_{i j} \leq|S|-1 \quad \forall S \subset N, 2 \leq|S| \leq n-1
$$

## Miller, Tucker, Zemling (MTZ) Formulation

$$
\begin{array}{lr}
\min \sum_{(i j) \in A} c_{i j} x_{i j} & \\
\sum_{i: i \neq j} x_{i j}=1 & \forall j=1, \ldots, n \\
\sum_{j: i \neq j} x_{i j}=1 & \forall i=1, \ldots, n \\
u_{i}-u_{j}+n x_{i j} \leq n-1, & \forall i, j=2,3, \ldots, n, i \neq j \\
x_{i j} \in \mathbb{B} & \forall i j \in A \\
u_{i} \in \mathbb{R} & \forall i=1, \ldots, n
\end{array}
$$

## Gavish-Graves (GG) Formulation

Single commodity flow. $g_{i j} \in \mathbb{R}^{+}$sequence variables (is 0 if $x_{i j}=0$ otherwise it indicates the number of arcs included on the path from vertex 1 up to $\operatorname{arc}(i, j)$ )

$$
\begin{array}{lr}
\min \sum_{(i j) \in A} c_{i j} x_{i j} & \forall j=1, \ldots, n \\
\sum_{i: i \neq j} x_{i j}=1 & \forall i=1, \ldots, n \\
\sum_{j: i \neq j} x_{i j}=1 & \\
\sum_{j=1}^{n} g_{j i}-\sum_{j=2}^{n} g_{i j}=1 & \forall i=2 . . n \\
g_{i j} \leq(n-1) x_{i j} & \forall i j \in A \\
x_{i j} \in \mathbb{B} & \forall i j \in A \\
g_{i j} \in \mathbb{R}^{+} & \forall i j \in A
\end{array}
$$

## Svestka (S) Formulation

- similar to precedent, also a single commodity flow formulation
- $y_{i j}$ : flow from city $i$ to city $j$
- $f$ : gain in flow from city $i$ to city $j$

$$
\begin{array}{lr}
\min \sum_{i j \in A} c_{i j} x_{i j} & \\
\sum_{j: j i \in A} y_{j i} \geq 1 & \forall i=2, \ldots, n \\
\sum_{j: j i j \in A} y_{i j}-\sum_{j: j i \in A} y_{j i}=f & \forall i=1, \ldots, n \\
\sum_{i j \in A} x_{i j} \leq n & \\
y_{i j} \leq(1+n f) x_{i j} & \forall i j \in A \\
x_{i j} \in \mathbb{B} & \forall i j \in A \\
y_{i j} \in \mathbb{R}^{+} & \forall i j \in A
\end{array}
$$

## Dantzig (D) Formulation

- Indices: $i, j k$ for cities, $t$ for step
- $x_{i j t}=1$ if we drive from city $i$ to city $j$ at step $t$, else 0 .

$$
\begin{array}{lr}
\min \sum_{i j \in A} \sum_{t} c_{i j} x_{i j t} & \\
\sum_{i} x_{i j t}-\sum_{k} x_{j, k, t+1}=0 & \forall j \text { and } t=1, \ldots, n \\
\sum_{j} \sum_{t} x_{i j t}=1 & \forall i=1, \ldots, n \\
x_{i j t} \in \mathbb{B} & \forall i j \in A, t \tag{24}
\end{array}
$$

Dual bounds

| Instance | DFJ | MTZ | Svestka | Dantzig |
| :--- | ---: | ---: | ---: | ---: |
| ran20points | 3182.2 | 2538.8 | 1087.7 | 2504.1 |
| dantzig42.dat |  | 2538.8 | 1032.8 | 2504.2 |
| berlin52.dat |  |  |  |  |
| bier127.dat |  |  |  |  |

## Comparing LP relaxations

Source: Oncan, Altinel, Laporte, A comparative analysis of several asymmetric traveling salesman problem formulations (2009)

A B A and $B$ are incomparable $\longleftarrow$ By the way... What does this mean?
$A \longrightarrow B B$ is better than $A$
$\Delta \longleftrightarrow$ B A and $B$ are equivalent
Dashed lines denote new relationships


Fig. 2. Relative strength of the 24 ATSP formulations

## Symmetric DFJ

- $E=\{i, j \mid i \in V, j \in V, i<j\}$
(TSPIP) min $\sum c_{i j} x_{i j}$

$$
\begin{aligned}
\text { s.t. } & \sum_{i j \in \delta(i)} x_{i j}+\sum_{j i \in \delta(i)} x_{j i}=2 \text { for all } i \in V \\
& \sum_{i j \in E(S)} x_{i j} \leq|S|-1 \text { for all } \emptyset \subset S \subset V, 2 \leq|S| \leq n-1 \\
& x_{i j} \in\{0,1\} \text { for all } i j \in E
\end{aligned}
$$

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## Lazy Constraint Approach to DFJ

- relax the set of sub-tour elimination constraints
- $\mathcal{S}=\{\emptyset \subset S \subset V\}$
- $\mathcal{S}^{\prime} \subset \mathcal{S}$
- relax the integrality constraint
(RTSPIP) $\quad \min \sum c_{i j} x_{i j}$

$$
\begin{array}{ll}
\text { s.t. } & \sum_{i j \in \delta(i)} x_{i j}+\sum_{j i \in \delta(i)} x_{j i}=2 \text { for all } i \in V \\
& \sum_{i j \in E(S)} x_{i j} \leq|S|-1 \text { for all } S \in \mathcal{S}^{\prime} \\
& x_{i j} \in\{0,1\} \text { for all } i j \in E
\end{array}
$$

$$
\begin{aligned}
(\text { RTSPLP }) & \min
\end{aligned} \begin{aligned}
& c_{i j} x_{i j} \\
\text { s.t. } & \sum_{i j \in \delta(i)} x_{i j}+\sum_{j i \in \delta(i)} x_{j i}=2 \text { for all } i \in V \\
& \sum_{i j \in E(S)} x_{i j} \leq|S|-1 \text { for all } S \in \mathcal{S}^{\prime} \\
& x_{i j} \in \mathbb{R}^{+} \text {for all } i j \in E
\end{aligned}
$$

## Implementation V1

```
set \(\mathcal{S}^{\prime}=\emptyset\)
    1. \(x^{*} \longleftarrow\) Solve \(\operatorname{RTSPIP}\left(\mathcal{S}^{\prime}\right)\)
    2. \(\mu_{k}, S \longleftarrow\) Solve \(\operatorname{SEP}\left(x^{*}\right)\)
        if \(\mu_{k}<2\) then set \(\mathcal{S}^{\prime}=\mathcal{S}^{\prime} \cup S\) and go to 1
        else return optimal solution \(x^{*}\)
```

SEP: connected components or number of cycles
In gurobi and cplex implementation via Lazy constraints (Model.cbLazy) and call back function called when MIPSOL. See script: tsp_gurobi_lazy

## Implementation V2

```
set \(\mathcal{S}=\emptyset\)
    1. \(x^{*} \longleftarrow\) Solve \(\operatorname{RLP}\left(\mathcal{S}^{\prime}\right)\)
    2. \(\mu_{k}, S \longleftarrow\) Solve \(\operatorname{SEPLP}\left(x^{*}\right)\)
        if \(\mu_{k}<2\) then set \(\mathcal{S}^{\prime}=\mathcal{S}^{\prime} \cup S\) and go to 1
        else go to 3
```

3. branch and bound and repeat 1 . and 2. at every node.

SEPLP: LP formulation or Max Flow
In gurobi and cplex implementation via Lazy constraints (Model.cbLazy) and call back functions when LP solution at node.

- Is the Asymmetric formulation TUM when all sub-tour elimination constraints are removed?
- Is the Symmetric formulation TUM when all sub-tour elimination constraints are removed?
- Does the DFJ formulation describe the convex hull of the problem?


## Traveling Salesman Problem

。14

- 15


19

$$
.21
$$

$$
20
$$

Figure 3.1 Locations of the 42 cities.

## Traveling Salesman Problem



Figure 3.2 Solution of the initial LP relaxation.

## Traveling Salesman Problem



Figure 3.3 LP solution after three subtour constraints.

## Traveling Salesman Problem



Figure 3.4 LP solution satisfying all subtour constraints.

## Traveling Salesman Problem



Figure 3.7 What is wrong with this vector?

## Traveling Salesman Problem



Figure 3.8 A violated comb.

## Traveling Salesman Problem



Figure 3.9 An optimal tour through 42 cities.

## An Improved DFJ Formulation. (why?)

$$
\begin{gathered}
\text { minimize } c^{\top} x \text { subject to } \\
0 \leq x_{e} \leq 1 \text { for all edges } e, \\
\sum\left(x_{e}: v \text { is an end of } e\right)=2 \text { for all cities } v, \\
\sum\left(x_{e}: e \text { has one end in } S \text { and one end not in } S\right) \geq 2 \\
\text { for all nonempty proper subsets } S \text { of cities, } \\
\sum_{i=0}^{i=3}\left(\sum\left(x_{e}: e \text { has one end in } S_{i} \text { and one end not in } S_{i}\right) \geq 10,\right. \\
\text { for any comb }
\end{gathered}
$$

## Comb inequalities

A comb can be defined by a handle $H$ and a number of teeth $T_{1}, T_{2}, \ldots, T_{s}$ such that:

- $H, T_{1}, T_{2}, \ldots, T_{s} \subseteq V$
- $T_{j} \backslash H \neq \emptyset \quad \forall 1 \leq j \leq s$
- $T_{j} \cap H \neq \emptyset \quad \forall 1 \leq j \leq s$
- $T_{i} \cap T_{j}=\emptyset \quad \forall i<j \leq s$
- $s \geq 3$ and odd

A comb inequality states that (in the two versions, of which only one is needed):

$$
\begin{aligned}
& x(\delta(H))+\sum_{j=1}^{s} x\left(\delta\left(T_{j}\right)\right) \geq 3 s+1 \quad \text { cut set constraints } \\
& x(E(H))+\sum_{j=1}^{s} x\left(E\left(T_{j}\right)\right) \leq|H|+\sum_{j=1}^{s}\left|T_{j}\right|-\frac{3 s+1}{2} \quad \text { subtour elimination constraints }
\end{aligned}
$$

Comb inequalities are valid inequalities for the TSP.

## 24,978 Cities

solved by LK-heuristic and prooved optimal by branch and cut

10 months of computation on a cluster of 96 dual processor Intel Xeon 2.8 GHz workstations
http://www.tsp.gatech.edu
sw24978 Branching Tree - Run 5


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