The Traveling Salesman Problem (TSP)

Overview

The Traveling Salesman Problem (TSP) is possibly *the* classic discrete optimization problem.

A preview :

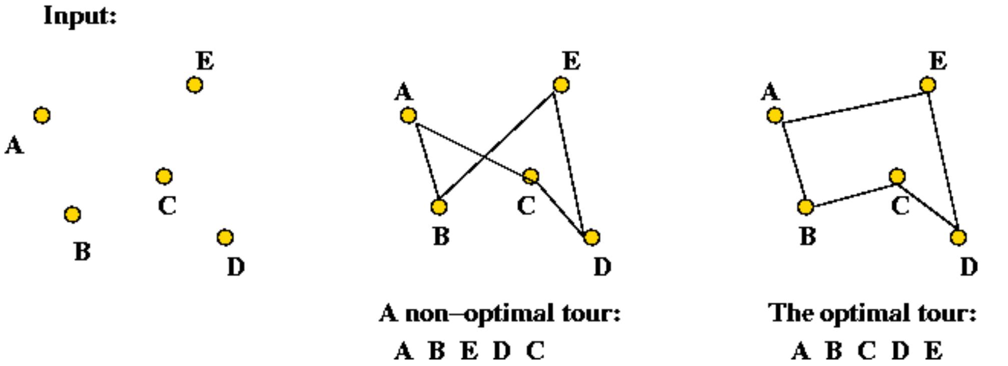
- How is the TSP problem defined?
- What we know about the problem: NP-Completeness.
- The construction heuristics: Nearest-Neighbor, MST, Clarke-Wright, Christofides.
- K-OPT.
- Simulated annealing and Tabu search.
- The Held-Karp lower bound.
- Lin-Kernighan.
- Lin-Kernighan-Helsgaun.
- Exact methods using integer programming.

Our presentation will pull together material from various sources - see the references below. But most of it will come from [Appl2006], [John1997], [CS153].

Defining the TSP

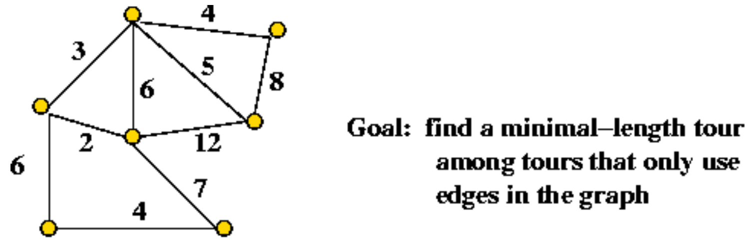
The TSP is fairly easy to describe:

- Input: a collection of points (representing cities).
- Goal: find a tour of minimal length.
  Length of tour = sum of inter-point distances along tour



- Details:
  - Input will be a list of n points, e.g., $(x_0, y_0), (x_1, y_1), ..., (x_{n-1}, y_{n-1})$.
  - Solution space: all possible tours.
  - "Cost" of a tour: total length of tour.
    → sum of distances between points along tour
  - Goal: find the tour with minimal cost (length).

- Strictly speaking, we have defined the *Euclidean TSP*.
- There are really three kinds:
  - The Euclidean (points on the plane).
  - The *metric* TSP: triangle inequality is satisfied.
  - The *graph* TSP:



Exercise:

- For an n-point problem, what is the size of the solution space (i.e., how many possible tours are there)?
- What's an example of an instance that's metric but not Euclidean?

Some assumptions and notation for the remainder:

- Let $n = |V|$ = number of vertices.
- Euclidean version, unless otherwise stated.
  → Complete graph.

Some history

Early history:

- 1832: informal description of problem in German handbook for traveling salesmen.
- 1883 U.S. estimate: 200,000 traveling salesmen on the road
- 1850's onwards: circuit judges

  Exercise: Find the following 14 cities in Illinois/Indiana on a map and identify the best tour you can:

  Bloomington, Clinton, Danville, Decatur, Metamora, Monticello, Mt.Pulaski, Paris, Pekin, Shelbyville, Springfield, Sullivan, Taylorville, Urbana

- 1960's: Proctor and Gamble $10K competition: a 33-city TSP.
  → Won by a CMU mathematician (and others).
- A related problem: the *Knight's tour*.
  → Start at bottom-left corner, and visit all squares exactly once and return to the start.

  Exercise: Show how the Knight's tour can be converted into a TSP instance.

- The statisticians take an interest
  → What is the expected length of an optimal tour for uniformly-generated points in 2D?
  - Several early analytic estimates in the 1940's.
  - Famous Beardwood-Halton-Hammersley result [Bear1959]:
    If L^* = optimal tour's length then $L^* / \sqrt{n} \rightarrow$ a constant β
  - β estimated to be 0.72 for unit-square.
- Human solutions:
  - To assess problem-solving skill.
  - Part of some neurological tests.

TSP's importance in computer science:

- TSP has played a starring role in the development of algorithms.
- Used as a test case for almost every new (discrete) optimization algorithm:
  - Branch-and-bound.
  - Integer and mixed-integer algorithms.
  - Local search algorithms.
  - Simulated annealing, Tabu, genetic algorithms.
  - DNA computing.

Some milestones:

- Best known optimal algorithm: Held-Karp algorithm in 1962, $O(n^2 2^n)$.
- Proof of NP-completeness: Richard Karp in 1972 [Karp1972].
  → Reduction from Vertex-Cover (which itself reduces from 3-SAT).
- Two directions for algorithm development:
  - Faster exact solution approaches (using linear programming).
    → Largest problem solved optimally: 85,900-city problem (in 2006).
  - Effective heuristics.
    → 1,904,711-city problem solved within 0.056% of optimal (in 2009)
- Optimal solutions take a long time
  → A 7397-city problem took three years of CPU time.
- Theoretical development: (let L_H = tour-length produced by heuristic, and let L^* be the optimal tour-length)
  - 1976: Sahni-Gonzalez result [Sahn1976]. Unless P=NP no polynomial-time TSP heuristic can guarantee $L_H/L^* \leq 2^{p(n)}$ for any fixed polynomial $p(n)$.
  - Various bounds on particular heuristics (see below).
  - 1992: Arora et al result [Aror1992]. Unless P=NP, there exists $\varepsilon>0$ such that no polynomial-time TSP heuristic can guarantee $L_H/L^* \leq 1+\varepsilon$ for all instances satisfying the triangle inequality.
  - 1998: Arora result [Aror1998]. For Euclidean TSP, there is an algorithm that is polyomial for fixed $\varepsilon>0$ such that $L^H/^{*}_H \leq 1+\varepsilon$

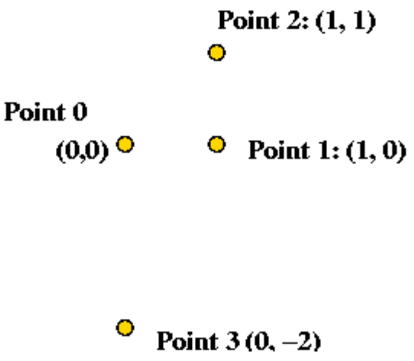
Approximate solutions: nearest neighbor algorithm

Nearest-neighbor heuristic:

- Possibly the simplest to implement.
- Sometimes called Greedy in the literature.
- Algorithm:

```
V = {1, ..., n-1}          // Vertices except for 0.
U = {0}                    // Vertex 0.
while V not empty
   u = most recently added vertex to U
   Find vertex v in V closest to u
   Add v to U and remove v from V.
endwhile
Output vertices in the order they were added to U
```

Exercise: What is the solution produced by Nearest-Neighbor for the following 4-point Euclidean TSP. Is it optimal?

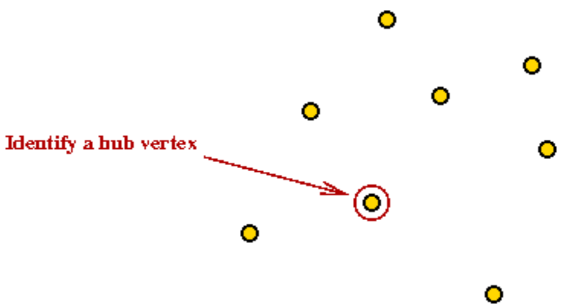


- What we know about Nearest-Neighbor:
  - $L_H/L^* \leq O(\log n)$
  - There are instances for which $L_H/L^* = O(\log n)$
  - There are sub-classes of instances for which Nearest-Neighbor consistently produces the *worst* tour [Guti2007].

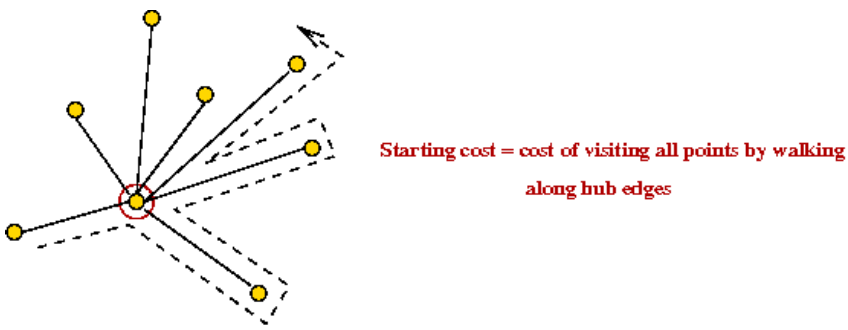
Approximate solutions: the Clarke-Wright heuristic

The Clarke-Wright algorithm: [Clar1964].

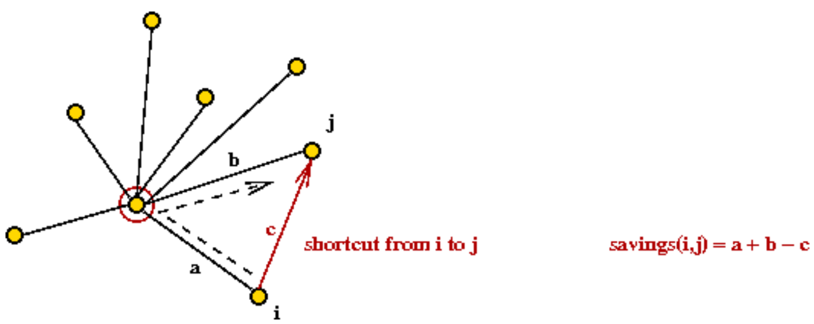
- The idea:
  - First identify a "hub" vertex:



  - Compute starting cost as cost of going through hub:



  - Identify "savings" for each pair of vertices:

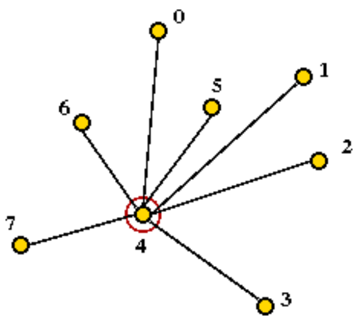


  - Take shortcuts and add them to final tour, as long as no cycles are created.

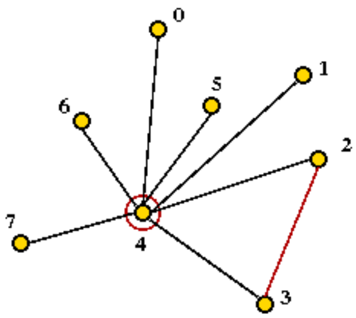
- Algorithm:

```
Identify a hub vertex h
V_H = V - {h}
for each i,j != h
   compute savings(i,j)
endfor
sortlist = Sort vertex pairs in decreasing order of savings
while |V_H| > 2
   try vertex pair (i,j) in sortlist order
   if (i,j) shortcut does not create a cycle
      and degree(v) ≤ 2 for all v
        add (i,j) segment to partial tour
        if degree(i) = 2
           V_H =  V_H - {i}
        endif
        if degree(j) = 2
           V_H =  V_H - {j}
        endif
   endif
endwhile
Stitch together remaining two vertices and hub into final tour
```

- Example (from above):
  - Suppose vertex 4 is the hub vertex:

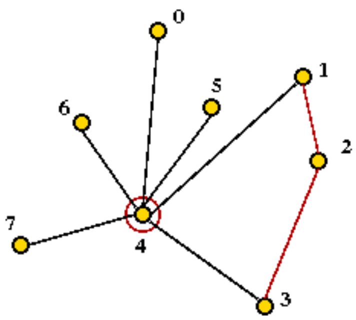


  - Suppose (2,3) provides the most savings:



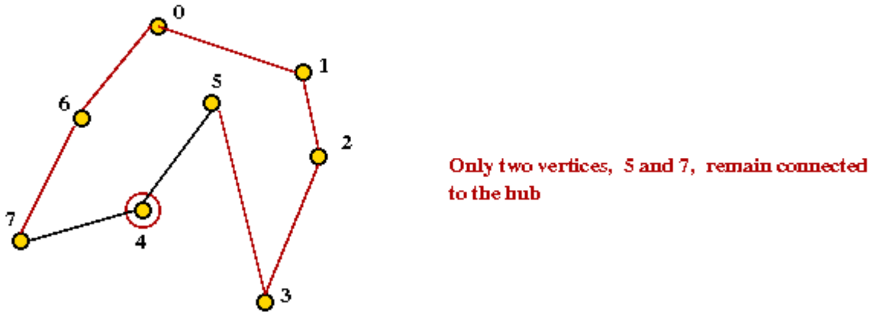
(2,3) gets added but no hub edge is removed (yet)

  - Next, (1,2) gets added
    → degree(2) = 2
    → must remove hub edge (2,4)

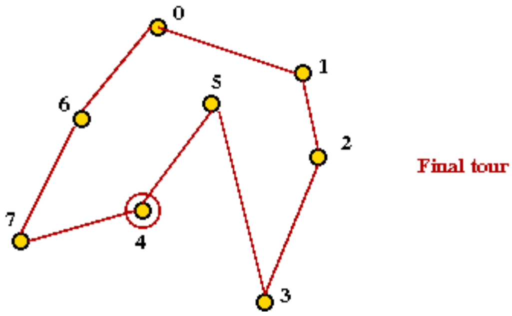


(1,2) is added and hub edge (2,4) is removed

- Continuing ... let's say we obtain:



- Finally, add last two vertices and hub into final tour:



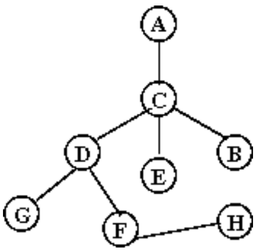
- What's known about the CW heuristic:
  - Bound is logarithmic: $L_H/L^* \leq O(log\ n)$
  - Worst examples known: $L_H/L^* \geq O(log(n) / loglog(n))$

Approximate solutions: the MST heuristic

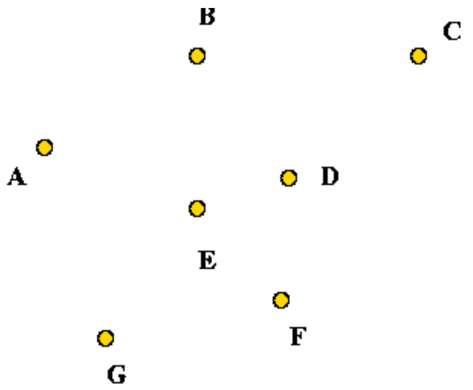
An approximation algorithm for (Euclidean) TSP that uses the MST: [Rose1977].

- The algorithm:
  1. First find the minimum spanning tree (using any MST algorithm).
  2. Pick any vertex to be the root of the tree.
  3. Traverse the tree in *pre-order*.
  4. Return the order of vertices visited in pre-order.

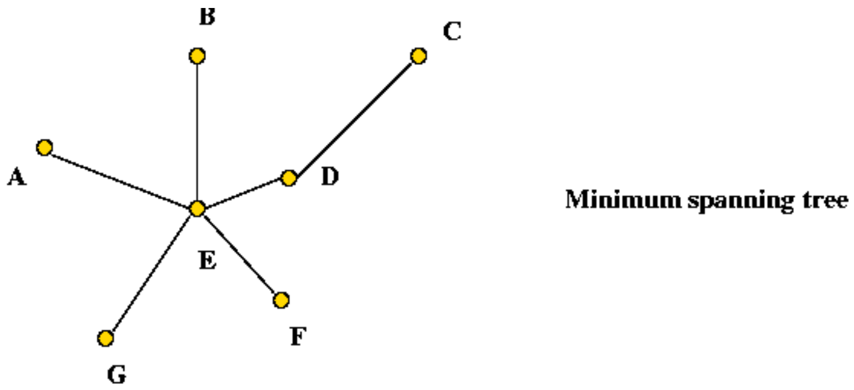
Exercise: What is the pre-order for this tree (starting at A)?



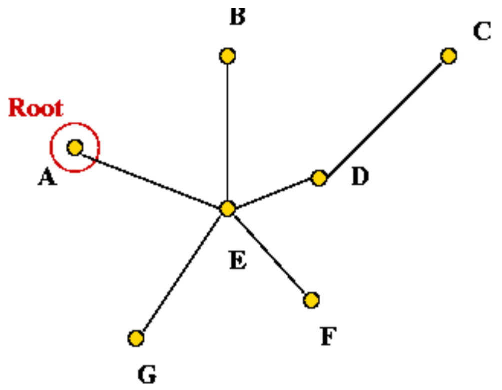
- Example:
  - Consider these 7 points:



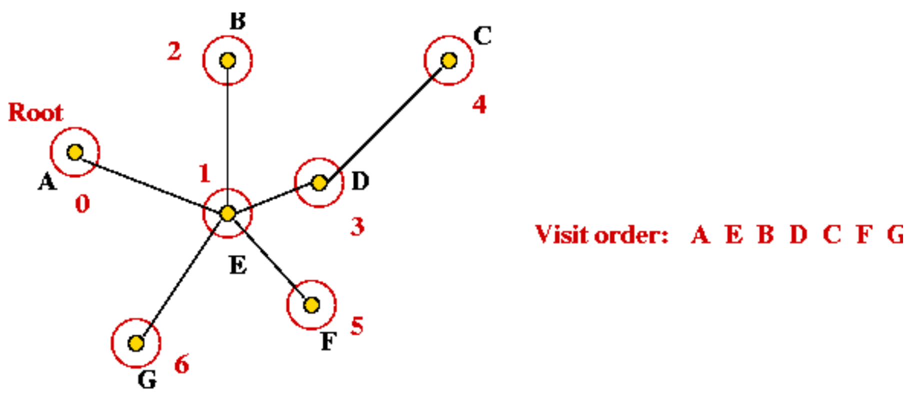
- A minimum-spanning tree:



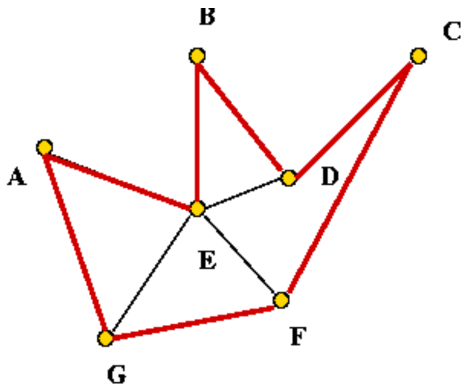
- Pick vertex A as the root:



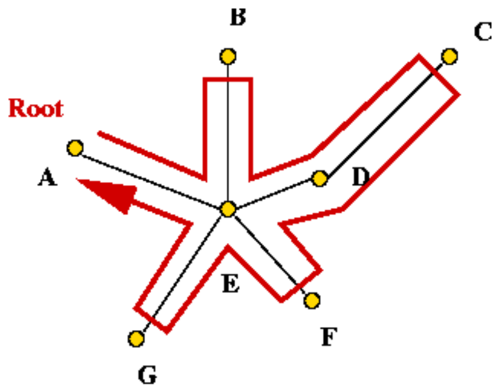
- Traverse in pre-order:



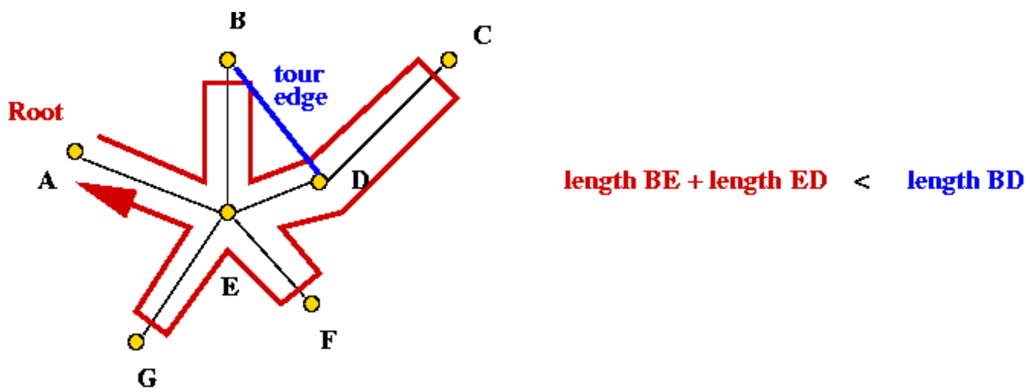
- Tour:



- Claim: the tour's length is no worse than twice the optimal tour's length.
  - Let L = the length of the tour produced by the algorithm.
  - Let L^* = the length of an optimal tour.
  - Let M = weight of the MST (total length).
  - Observe: if we remove any one edge from a tour, we will get a spanning tree.
    $\rightarrow L^* > M$.
  - Now consider a pre-order *tree walk* from the root, back to the root:



  - Let W = length of this walk.
  - Then, $W = 2M$ (each edge is traversed twice).
  - Thus, $W < 2L^*$.
  - Finally, we will show that $L \le W$ and therefore, $L < 2L^*$.
  - To see why, consider the tree walk from B to D:



$\rightarrow$ L takes a shorter route than W (triangle inequality).

  - Thus, $L \le W$.

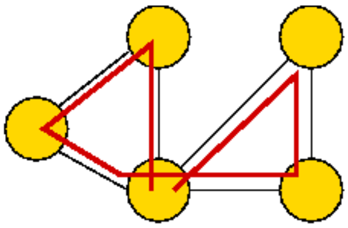
What we know about this algorithm:

- The first heuristic to produce solutions within a constant of optimal.
- Easy to implement (since MST can be found efficiently).

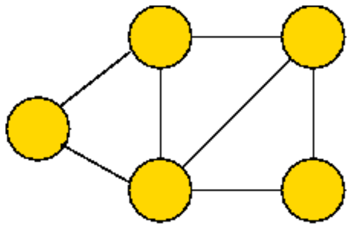
Approximate solutions: the Christofides heuristic

The Christofides algorithm: [Chri1976].

- First, as background, we need to understand two things:
  - What is an Euler tour (for general graphs)?
    → A tour that traverses all edges exactly once (but may repeat vertices)

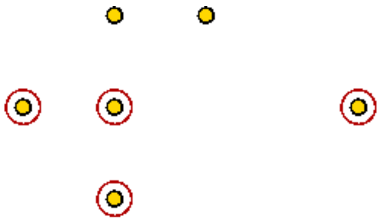


Euler tour exists

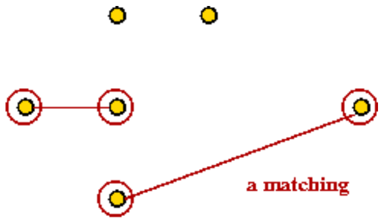


No Euler tour possible

  - Famous result: a graph has an Euler tour if and only if all its vertices have even degree.
  - What is a minimal matching for a given subset of vertices V'?
    → A "best" (minimal weight) subset of edges with the property that no edges have a common vertex

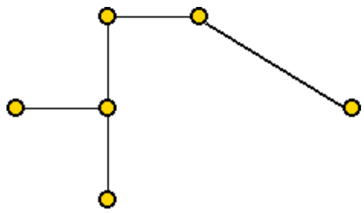


V' = given set of vertices for which matching is desired

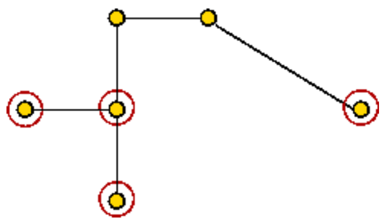


  - Important result: min-matching can be found in poly-time.

- The key ideas in the algorithm:
  - First find the MST



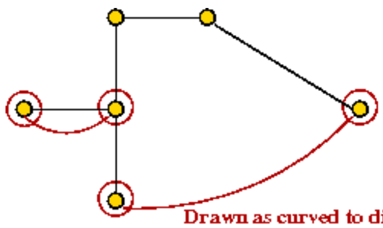
  - Then identify the odd-degree vertices



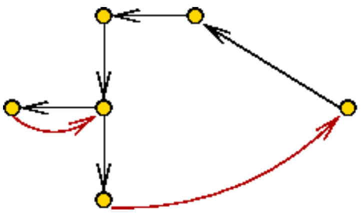
  - There are an *even* number of such odd-degree vertices.

    Exercise: Why?

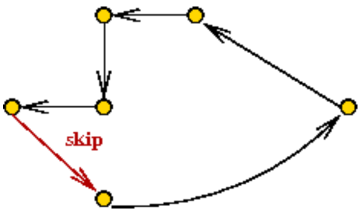
  - Find a minimal matching of these odd-degree vertices and add those edges



- Now all vertices have even degree.
- Next, find an Euler tour.



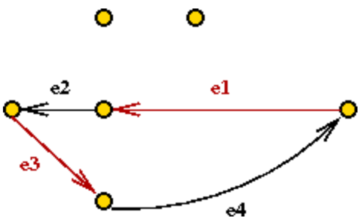
- Now, walk along in Euler tour, but skip visited nodes



- This produces a TSP tour.

An improved bound:

- We will show that $L_H/L^* \leq 1.5$
- Let M = cost of MST.
  $\rightarrow L^* \geq M$ (as argued before).
- Note: we are performing a matching on an even number of vertices.
- Now consider the original odd-degree vertices



  - Consider the optimal tour on just these (even # of) vertices.
  - Let L_O = cost of this tour.
  - Let $e^1, e^2, ..., e^{2k}$ be the edges.
  - Note: $E_1 = \{e^1, e^3, ..., e^{2k-1}\}$ is a matching.
  - So is $E_2 = \{e^2, e^4, ..., e^{2k}\}$
- Now at least one set has weight at most $L_O/2$.
  $\rightarrow$ Because both must add up to L_O.
- Also the optimal matching found earlier has less weight than either of these edge sets.
  $\rightarrow$ min-match-cost $\leq L_O/2 \leq L^*/2$.
- Thus min-match-cost + $M \leq L^* + L^*/2$
- But L_H uses edges (or shortcuts) from min-match and MST

→ $L_H \leq L^* + L^*/2$

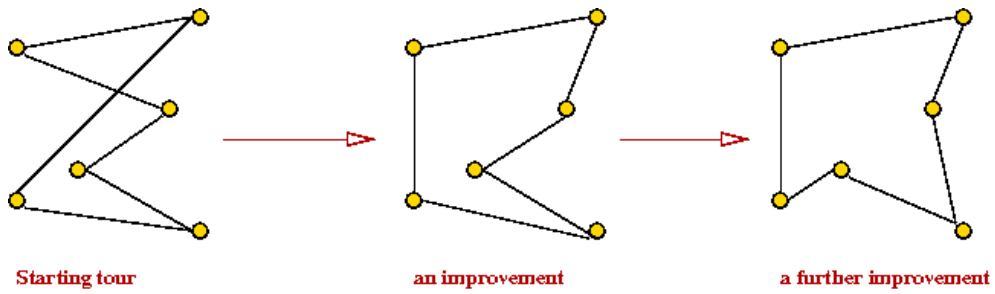
Running time:

- Dominated by $O(n^3)$ time for matching.
- Best known matching algorithm: $O(n^{2.376})$

K-OPT

Constructive vs. local-search heuristics:

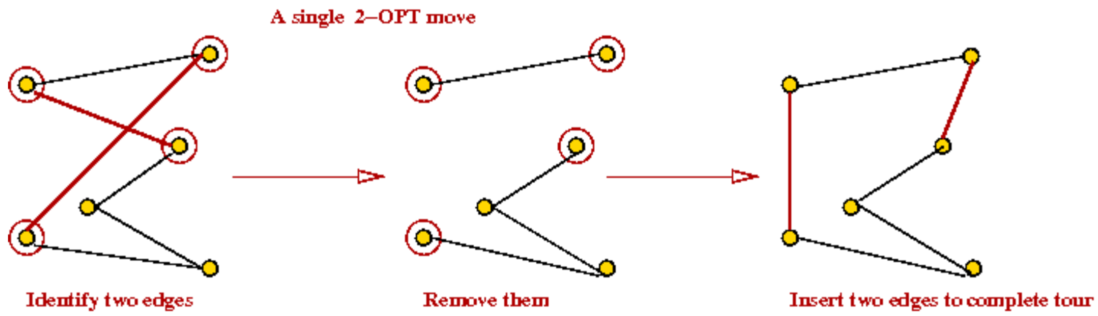
- All four heuristics above were *constructive*
  → A tour was built up step by step.
- In contrast, a local-search heuristic works as follows:




```
T = some starting tour      // Perhaps by using Christofides.
noChange = true
repeat
   T' = makeChangeTo (T)
   if T' < T
       T = T'
       noChange = false
   endif
until noChange
return T
```

2-OPT:

- Idea: Replace 2 edges and see if the cost improves.



  - Find two edges and their endpoints.
  - Swap endpoints.

- 2-OPT heuristic

```
T = some starting tour
noChange = true
repeat
   for all possible edge-pairs in T
      T' = tour by swapping end points in edge-pair
      if T' < T
          T = T'
```

```
                noChange = false
                break      // Quit loop as soon as an improvement is found
            endif
        endfor
    until noChange
    return T
```

- An alternative: find best tour with all possible swaps:

```
T = some starting tour
noChange = true
repeat
   T_best = T
   for all possible edge-pairs in T
      T' = tour by swapping end points in edge-pair
      if T' < T_best
          T_best = T'
          noChange = false
      endif
   endfor
   T = T_best
until noChange
return T
```

K-OPT:

- 3-OPT is what you can get by considering replacing 3 edges.
- K-OPT considers K edges.
- Each K-OPT can be time-consuming for K > 3.

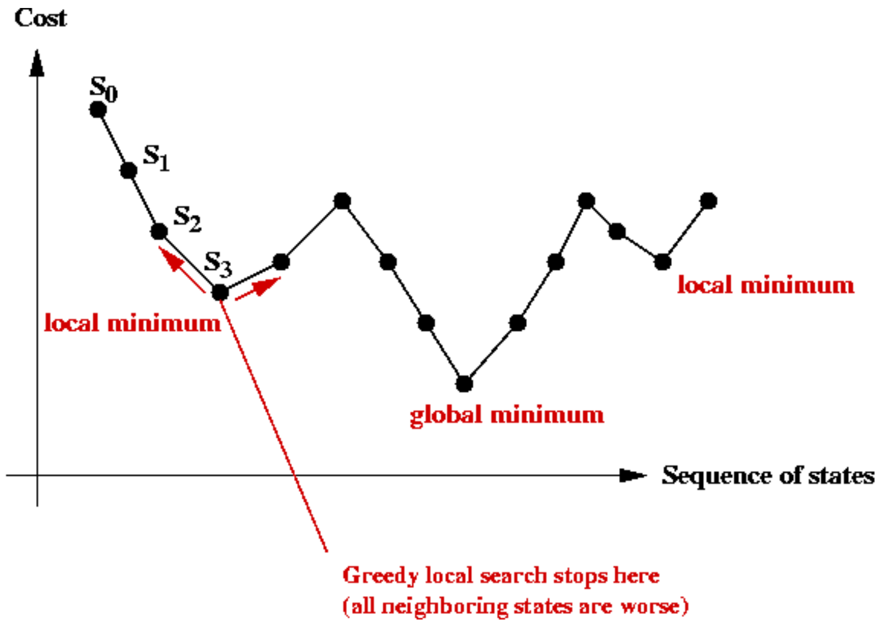
What we know about K-OPT:

- For general graphs: $L_H/L^* \leq 0.25\ n^{1/2k}$.
- For Euclidean case, $L_H/L^* \leq O(\log n)$.
- In practice: 2-OPT and 3-OPT are much better than the construction heuristics.
- Note: Any K-OPT move can be reduced to a sequence of 2-OPT moves.
  → But might it might require a long such sequence.

Local Optima and Problem Landscape

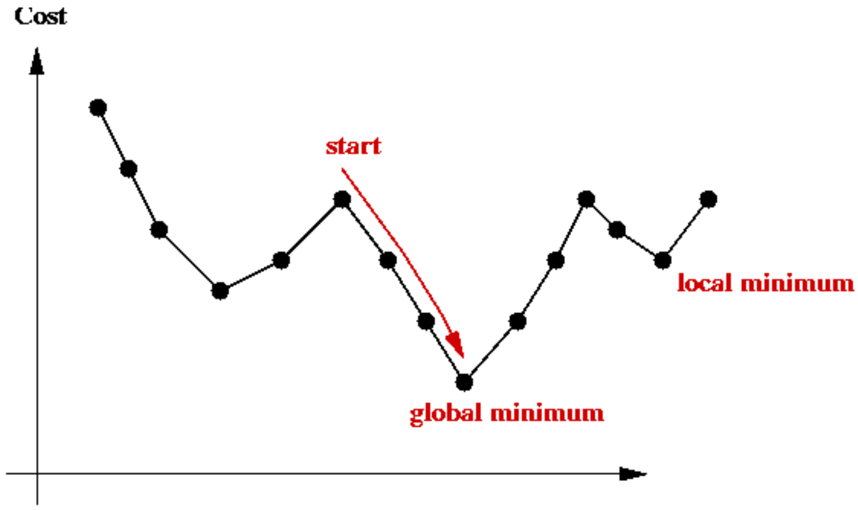
Local optima:

- Recall: greedy-local-search generates one state (tour) after another until no better neighbor can be found
  → does this mean the last one is optimal?
- Observe the trajectory of states:



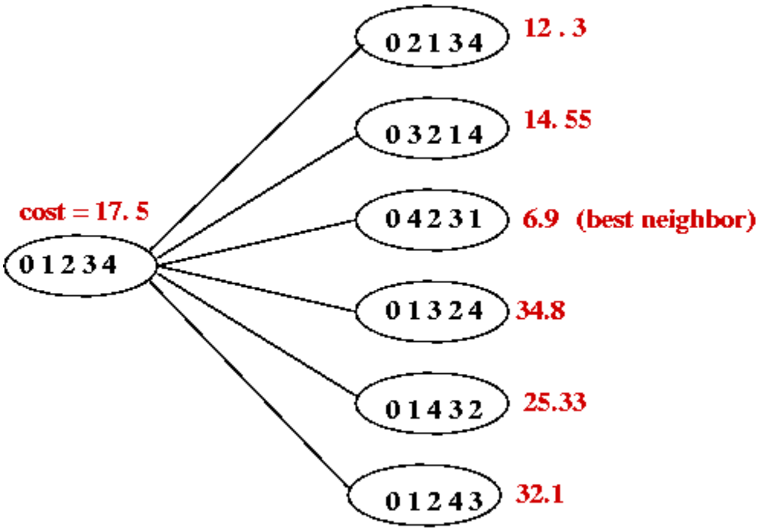
- There is no guarantee that a greedy local search can find the (global) minimum.

- The last state found by greedy-local-search is a *local minimum*.
  → it is the "best" in its neighborhood.
- The *global minimum* is what we seek: the least-cost solution overall.
- The particular local minimum found by greedy-local-search depends on the start state:



Problem landscape:

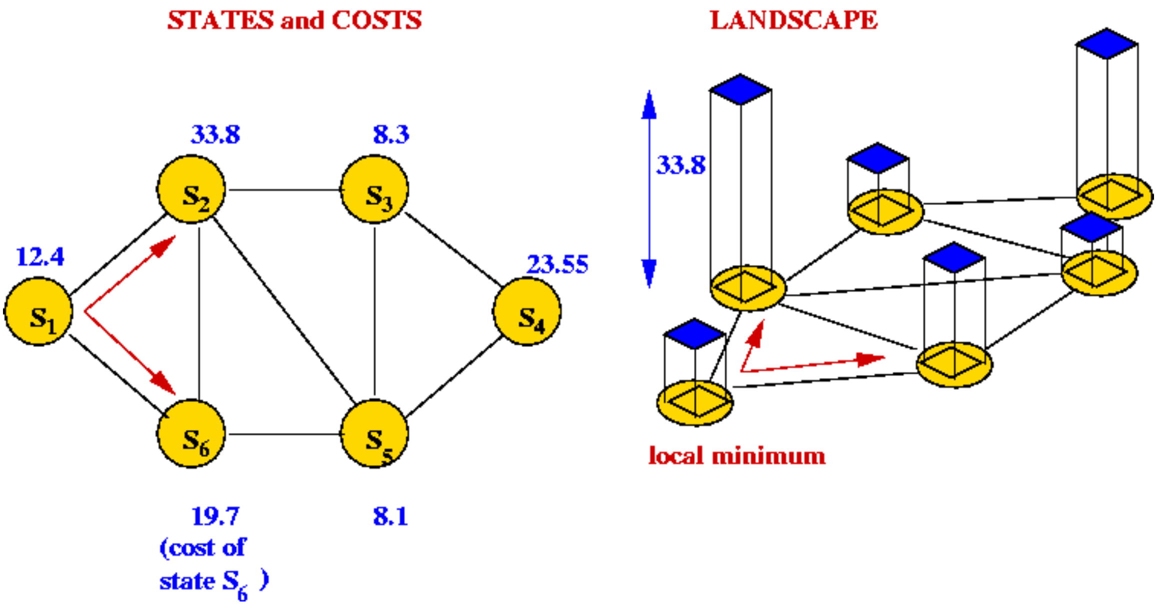
- Consider TSP using a particular local-search algorithm:
  - Suppose we use a graph where the vertices represent states.
  - An edge is placed between two "neighbors"
    e.g., for a 5-point TSP the neighbors of [0 1 2 3 4] are:



Neighbors of [0 1 2 3 4] using a 2–point swap

- The cost of each tour is represented as the "weight" of each vertex.
- Thus, a local-search algorithm "wanders" around this graph.

- Picture a 3D surface representing the cost *above* the graph.
→ this is the problem landscape for a particular problem and local-search algorithm.



- A large part of the difficulty in solving combinatorial optimization problems is the "weirdness" in landscapes
→ landscapes often have very little structure to exploit.

- Unlike continuous optimization problems, local shape in the landscape does NOT help point towards the global minimum.

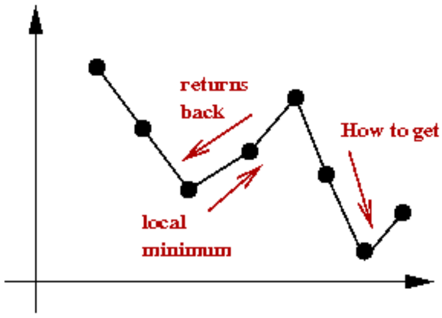
Climbing out of local minima:

- A local-search algorithm gets "stuck" in a local minimum.
- One approach: re-run local-search many times with different starting points.
- Another approach (next): help a local-search algorithm "climb" out of local minima.

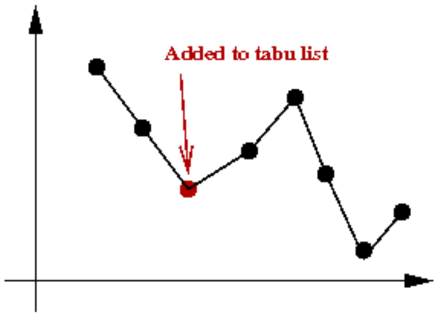
Tabu search

Key ideas: [Glov1990].

- Suppose we decide to climb out of local minima.
- Danger: could immediately return to same local minima.



- In tabu-search, you maintain a list of "tabu tours".
  → The algorithm avoids these.
- Each time you pick a minimum in a neighborhood, add that to the tabu list.

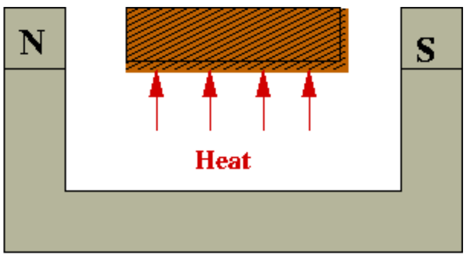


- Various alternatives to tabu-lists
  - Always add all neighborhood minimums.
  - Only add local minima.
- This way, Tabu forces more searching.
- A problem: a tabu-list can grow very long.
  → Need a *policy* for removing items, e.g.,
  - Least-recently used.
  - Throw out high-cost tours.

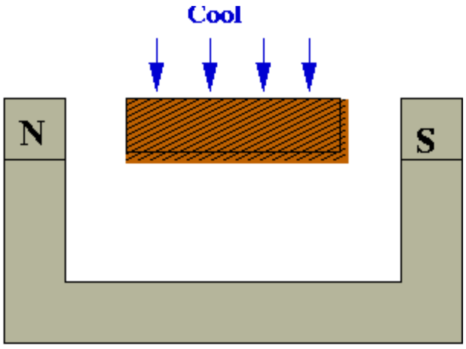
Simulated annealing

Background:

- What is *annealing*?
  - *Annealing* is a metallurgic process for improving the strength of metals.
  - Key idea: cool metal slowly during the forging process.
- Example: making bar magnets:
  - Wrong way to make a magnet:
    1. Heat metal bar to high temperature in magnetic field.

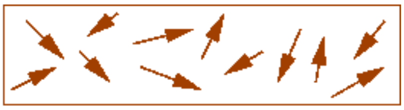


2. Cool rapidly (quench):

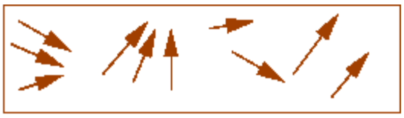


- Right way: cool slowly (anneal)

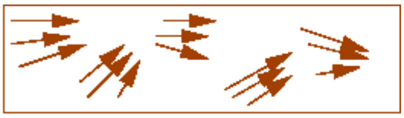
- Why slow-cooling works:
  - At high heat, magnetic dipoles are agitated and move around:



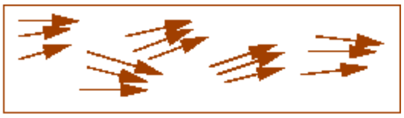
  - The magnetic field tries to force alignment:



  - If cooled rapidly, alignments tend to be less than optimal (local alignments):



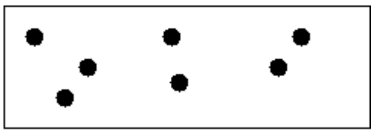
  - With slow-cooling, alignments are closer to optimal (global alignment):



- Summary: slow-cooling helps because it gives molecules more time to "settle" into a globally optimal configuration.

- Relation between "energy" and "optimality"
  - The more aligned, the lower the system "energy".
  - If the dipoles are not aligned, some dipoles' fields will conflict with others.
  - If we (loosely) associate this "wasted" conflicting-fields with energy
    $\rightarrow$ better alignment is equivalent to lower energy.
  - Global minimum = lowest-energy state.

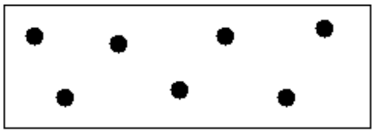
- The Boltzmann Distribution:
  - Consider a gas-molecule system (chamber with gas molecules):



  - The state of the system is the particular snapshot (positions of molecules) at any time.
  - There are high-energy states:

High–energy: molecules bunched up

and low-energy states:



Low energy state: molecules spread apart

- Suppose the states s_1, s_2, ... have energies $E(s_1)$, $E(s_2)$, ...
- A particular energy value E occurs with probability

  $$P[E] = Z\, e^{-E/kT}$$

  where Z and k are constants.

- Low-energy states are more probable at low temperatures:
  - Consider states s_1 and s_2 with energies $E(s_2) > E(s_1)$
  - The ratio of probabilities for these two states is:

  $$r = P[E(s_1)] / P[E(s_2)] = e^{[E(s_2) - E(s_1)] / kT} = exp\ ([E(s_2) - E(s_1)] / kT)$$

Exercise : Consider the ratio of probabilities above:

- Question: what happens to r as T increases to infinity?
- Question: what happens to r as T decreases to zero?

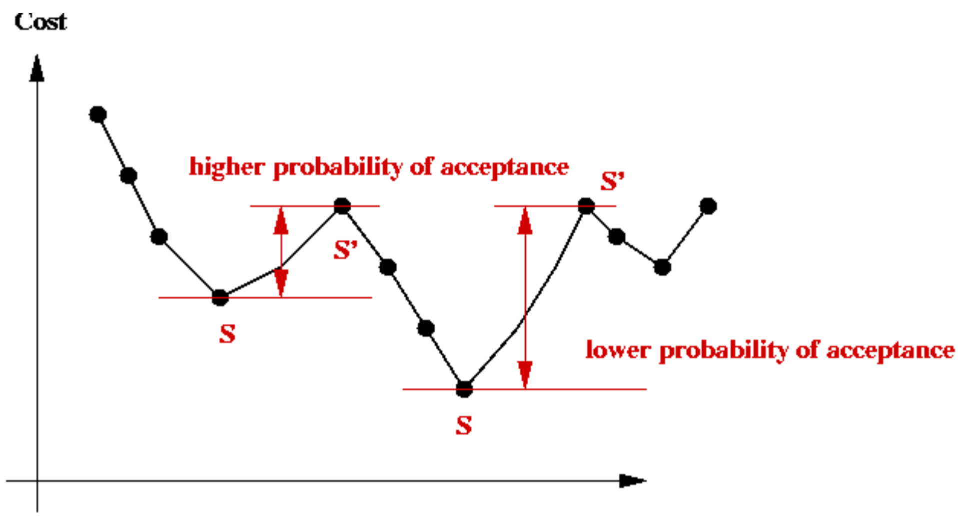
What are the implications?

Key ideas in simulated annealing: [Kirk1983].

- Simulated annealing = a modified local-search.
- Use it to solve a combinatorial optimization problem.
- Associate "energy" with "cost".
  → Goal: find lowest-energy state.
- Recall problem with local-search: gets stuck at local minimum.
- Simulated annealing will allow jumps to higher-cost states.
- If randomly-selected neighbor has lower-cost, jump to it (like local-search does).
- If randomly-selected neighbor is of higher-cost
  → flip a coin to decide whether to jump to higher-cost state
  - Suppose current state is s with cost $C(s)$.
  - Suppose randomly-selected neighbor is s' with cost $C(s') > C(s)$.
  - Then, jump to it with probability

  $$e^{-[C(s') - C(s)] / kT}$$

- Decrease coin-flip probability as time goes on:
  → by decreasing temperature T.
- Probability of jumping to higher-cost state depends on cost-difference:



Prob[accept] = $\exp[-(C(s') - C(s))/T]$

Implementation:

- Pseudocode: (for TSP)

```
Algorithm: TSPSimulatedAnnealing (points)
Input: array of points

     // Start with any tour, e.g., in input order
     s = initial tour 0,1,...,n-1

     // Record initial tour as best so far.
     min = cost (s)
     minTour = s

     // Pick an initial temperature to allow "mobility"
     T = selectInitialTemperature()

     // Iterate "long enough"
     for i=1 to large-enough-number
           // Randomly select a neighboring state.
           s' = randomNextState (s)
           // If it's better, then jump to it.
           if cost(s') < cost(s)
               s = s'
               // Record best so far:
               if cost(s') < min
                   min = cost(s')
                   minTour = s'
               endif
           else if expCoinFlip (s, s')
               // Jump to s' even if it's worse.
               s = s'
           endif       // Else stay in current state.
           // Decrease temperature.
           T = newTemperature (T)
     endfor

     return minTour

Output: best tour found by algorithm



Algorithm: randomNextState (s)
Input: a tour s, an array of integers

    // ... Swap a random pair of points ...
```

```
Output: a tour


Algorithm: expCoinFlip (s, s')
Input: two states s and s'

p = exp ( -(cost(s') - cost(s)) / T)
u = uniformRandom (0, 1)
if u < p
    return true
else
    return false

Output: true (if coinFlip resulted in heads) or false
```

- Implementation for other problems, e.g., BPP
  - The only thing that needs to change: define a `nextState` method for each new problem.
  - Also, some experimentation will be need for the temperature schedule.

Temperature issues:

- Initial temperature:
  - Need to pick an initial temperature that will accept large cost increases (initially).
  - One way:
    - Guess what the large cost increase might be.
    - Pick initial T to make the probability 0.95 (close to 1).
- Decreasing the temperature:
  - We need a *temperature schedule*.
  - Several standard approaches:
    - Multiplicative decrease: Use $T = a * T$, where a is a constant like 0.99.
      $\rightarrow T_n = a^n$.
    - Additive decrease: Use $T = T - a$, where a is a constant like 0.0001.
    - Inverse-log decrease: Use $T = a / log(n)$.
  - In practice: need to experiment with different temperature schedules for a particular problem.

Analysis:

- How long do we run simulated annealing?
  - Typically, if the temperature is becomes very, very small there's no point in further execution
    → because probability of escaping a local minimum is miniscule.
- Unlike previous algorithms, there is no fixed running time.
- What can we say theoretically?
  - If the inverse-log schedule is used
    → Can prove "probabilistic convergence to global minimum"
    → Loosely, as the number of iterations increase, the probability of finding the global minimum tends to 1.

In practice:

- Advantages of simulated annealing:
  - Simple to implement.
  - Does not need much insight into problem structure.
  - Can produce reasonable solutions.
  - If greedy does well, so will annealing.
- Disadvantages:
  - Poor temperature schedule can prevent sufficient exploration of state space.
  - Can require some experimentation before getting it to work well.

- Precautions:
  - Always re-run with several (wildly) different starting solutions.
  - Always experiment with different temperature schedules.
  - Always pick an initial temperature to ensure high probability of accepting a high-cost jump.
  - If possible, try different neighborhood functions.
- *Warning*:
  - Just because it has an appealing origin, simulated annealing is not guaranteed to work
    → when it works, it's because it explores more of the state space than a greedy-local-search.
  - Simply running greedy-local-search on multiple starting points may be just as effective, and should be experimented with.

Variations:

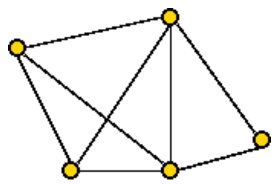
- Use greedyNextState instead of the nextState function above.
  - Advantage: guaranteed to find local minima.
  - Disadvantage: may be difficult or impossible to climb out of a particular local minimum:
    - Suppose we are stuck at state *s*, a local minimum.
    - We probabilistically jump to *s*', a higher-cost state.
    - When in *s*', we will very likely jump back to *s* (unless a better state lies on the "other side").
  - Selecting a random next-state is more amenable to exploration.
    → but it may not find local minima easily.
- Hybrid nextState functions:
  - Instead of considering the entire neighborhood of 2-swaps, examine some fraction of the neighborhood.
  - Switch between different neighborhood functions during iteration.
- Maintain "tabu" lists:
  - To avoid jumping to states already seen before, maintain a list of "already-visited" states and exclude these from each neighborhood.
- Thermal cycling:
  - Periodically raise temperature and perform "re-starts".
  - The idea is to force more exploration of the state space.

The Held-Karp lower bound

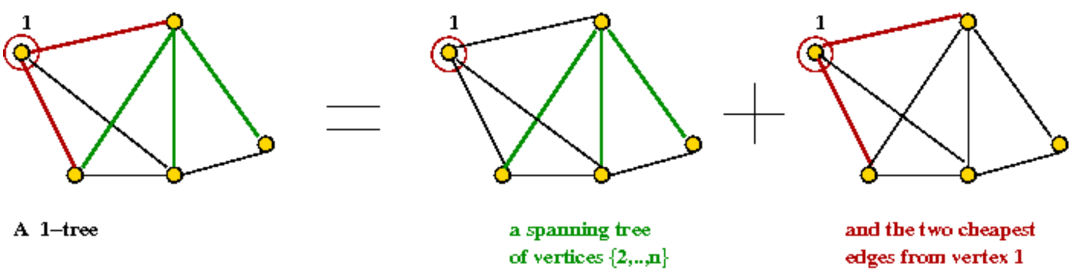
Our presentation will follow the one in [Vale1997].

First, a definition:

- Consider a graph with vertices *{1,...,n}*:

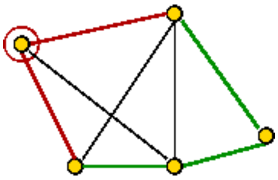


- A *1-tree* is a subgraph constructed as follows:



- Temporarily remove vertex 1 (and its edges) and find a spanning tree for vertices *{2,..,n}*.
- Then pick add two cheapest edges from vertex 1.

- Note: every tour (including the optimal one) is a 1-tree.

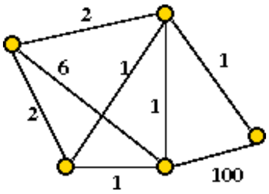


- The *min-1-tree* is the lowest weighted 1-tree among all 1-trees.
  → This will be a lower bound for the optimal tour.

- A simple algorithm for the min-1-tree:
  - Find the MST for the graph without vertex 1.
  - Add the two cheapest edges from vertex 1.

- Is the min-1-tree a good bound?

  Exercise: What is the difference between the optimal tour and the min-1-tree for this graph?



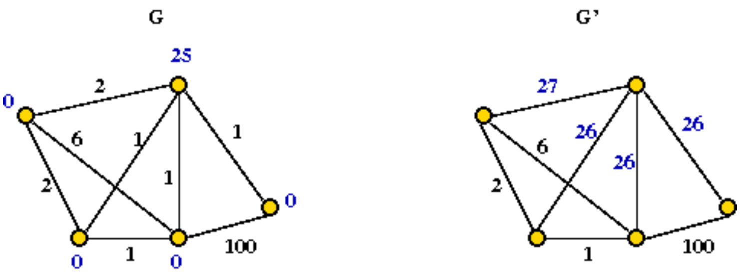
- The problem is: the MST can avoid using edges that the tour must take.

Held-Karp's idea:

- We will associate a π_i, a *vertex weight* with every vertex *i*.

- Define a modifed graph *G'* as follows:
  - *G'* has the same vertices and edges as *G*.
  - Let e_{ij} = weight of edge *(i,j)* in *G*.
  - Let c_{ij} = weight of edge *(i,j)* in *G'*.
  - Then define $c_{ij} = e_{ij} + \pi_i + \pi_j$.

- For example:



  Exercise: What is the difference between the min-1-tree and the optimal tour for the above modified graph *G'*? What vertex weight for the top-right vertex best closes the gap between the min-1-tree and the optimal tour?

- Thus, one can *choose* weights so that the min-1-tree is as high as possible in G'.

In more detail:

- Let *T* be a 1-tree and *T'* be a tour.

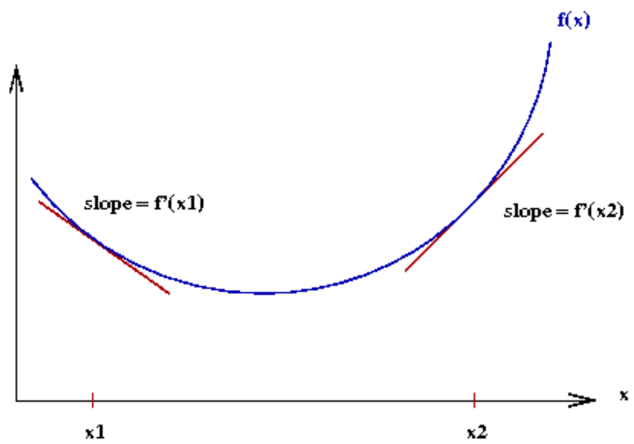
- Let $d^T{}_i$ = the degree of node i in T.
- Let $L(T,G)$ = cost of 1-tree T using graph G.
- Let $L(T',G)$ = cost of tour T' using graph G.
- Since every tour is a 1-tree, $min_T\ L(T,G) \leq min_{T'}\ L(T',G)$.
- Now, for a 1-tree T,
  $L(T,G') = L(T,G) + \Sigma_{i \varepsilon T}\ (d_i^T)\pi_i$.
- Similarly, for a tour T',
  $L(T',G') = L(T',G) + \Sigma_{i \varepsilon T'}\ 2\pi_i$.
- Thus, subtracting and taking minimum, $min_T\ L(T,G) + \Sigma_{i \varepsilon T}\ (d_i^T\text{-}2)\pi_i\ \ \leq\ \ min_{T'}\ L(T',G) = L^*$ (the optimal tour).
- To summarize, we want to find the min-1-tree with weights π and then correct for that by subtracting off the additional weights.
- Let $W(\pi) = min_T\ L(T,G) + \Sigma_{i \varepsilon T}\ (d_i^T\text{-}2)\pi_i$.
- Then, the desired "best" Held-Karp bound is: $max_\pi\ W(\pi)$.

An optimization procedure:

- Let $V_{T(\pi)}$ be the vector $(d^T{}_1, ..., d^T{}_n)$.
- Let $C_{T(\pi)}$ be the cost of min-1-tree using π.
- Then, write $W(\pi) = C_{T(\pi)} + \pi\ V_{T(\pi)}$.
- Next, suppose that π' is a vector in π-space such that $W(\pi') \geq W(\pi)$.
- Then, Held-Karp show that $(\pi' - \pi)\ V_{T(\pi)} \geq 0$.
- This means that larger values of $W(\pi')$ are in the right half-space pointed to by the vector $V_{T(\pi)}$.
- Next step: an iterative optimization procedure.

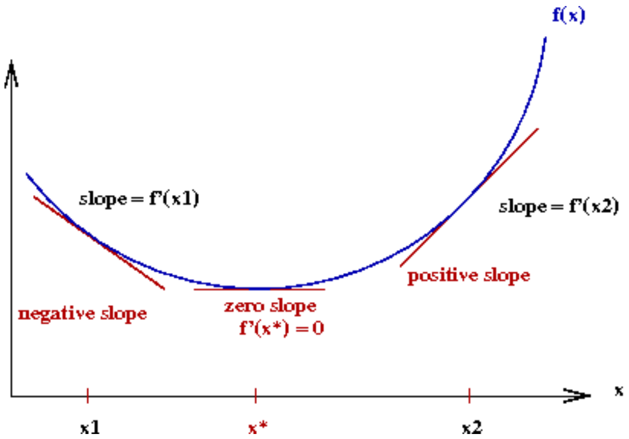
First, a little background on gradient-based optimization:

- Consider a (single-dimensional) function $f(x)$:



  - Let $f'(x)$ denote the derivative of $f(x)$.
  - The gradient at a point x is the value of $f'(x)$.
    → Graphically, the slope of the tangent to the curve at x.

- Observe the following:



  - To the left of the optimal value x^*, the gradient is negative.
  - To the right, it's positive.

- We seek an iterative algorithm of the form

```
while not over
    if gradient < 0
        move rightwards
    else if gradient > 0
        move leftwards
    else
        stop                // gradient = 0 (unlikely in practice, of course)
    endif
endwhile
```

- The gradient descent algorithm is exactly this idea:

```
while not over
    x = x - α f'(x)
endwhile
```

  Here, we add a scaling factor α in case $f'(x)$ values are of a different order-of-magnitude:

Back to vertex-weight optimization:

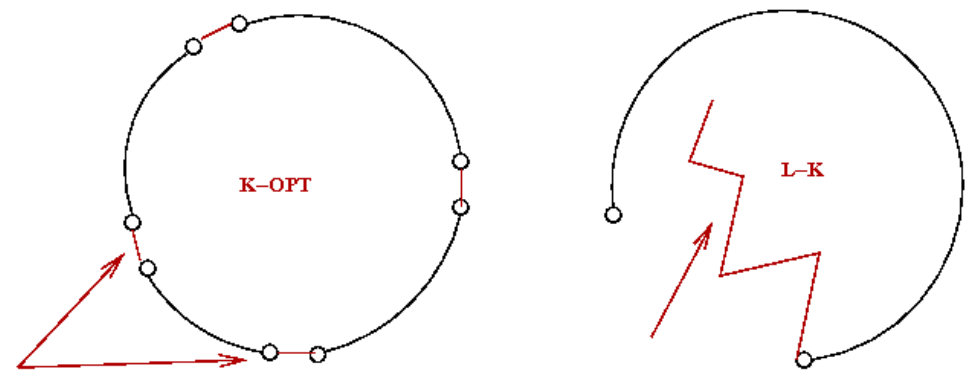
- Unfortunately, we don't have a differentiable function.
- For this case, the Russian mathematician Polyak devised what's called the *sub-gradient* algorithm:
  - For a differentiable function, the gradient "points" in the right direction.
  - For a non-differentiable function, it's still possible to use a gradient that points in the right direction.
- For the vertex-weights, the iteration turns out to be: $\pi_i^{(m+1)} = \pi_i^{(m)} + \alpha^{(m)} (d_i - 2)$.
- Intuitively, this means:
  - Increase the weights for vertices with 1-min-tree degree > 2.
  - Decrease the weights for vertices with 1-min-tree degree < 2.
  - Thus, the iteration tries to force the 1-min-tree to be "tour-like".
- Polyak showed that sub-gradient iteration works if the stepsizes $\alpha^{(m)}$ are chosen properly:
  - $\alpha^{(m)} \rightarrow 0$
  - $\sum_m \alpha^{(m)} = \infty$
- To summarize:
  - Start with some vector of vertex-weights π.
  - Repeatedly apply the iteration $\pi_i^{(m+1)} = \pi_i^{(m)} + stepsize * sub\text{-}gradient\ V_{T(\pi)}$.

- Implementation issues:
  - Each iteration requires an MST computation.
    → Can be expensive for large n.
  - One approximation: reduce number of edges by considering only best k neighbors (e.g., k=20).

The Lin-Kernighan algorithm

Key ideas:

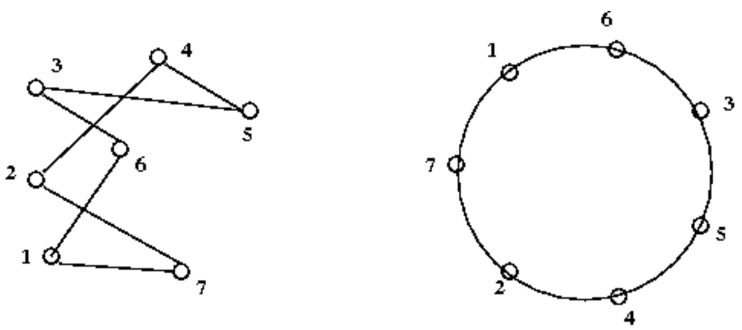
- Devised in 1973 by Shen Lin (co-author on BB(N) numbers) and Brian Kernighan (the "K" of K&R fame).
- Champion TSP heuristic 1973-89.
- LK is iterative:
  → Starts with a tour and repeatedly improves, until no improvement can be found.
- Idea 1: Make the K edges in K-OPT *contiguous*



K–OPT can pick edges anywhere L–K makes a contiguous path out of "edges in play"

  - This is just the high-level idea
    → The algorithm actually alternates between a "current-tour-edge" and a "new-putative-edge".
- Let the K in K-OPT vary at each iteration.
  - Try to increase K gradually at each iteration.
  - Pick the best K (the best tour) along the way.
- Allow some limited backtracking.
- Use a tabu-list to create freshness in exploration.

Note: we will use an artificial depiction of a tour as follows:

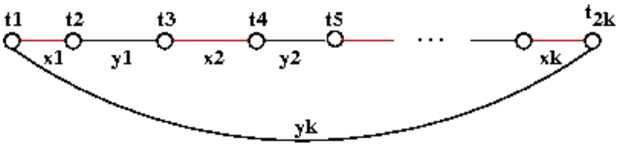


Actual graph and tour Circular visualization of tour

This will be used to explain some ideas.

The LK algorithm in more detail:

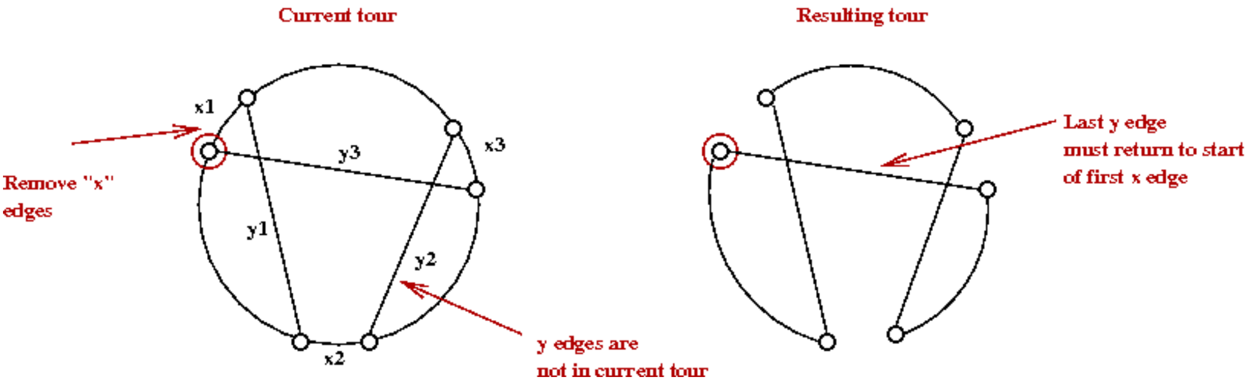
- At each iteration, LK identifies a sequence of edges x_1, y_1, x_2, y_2, ..., x_k, y_k such that:



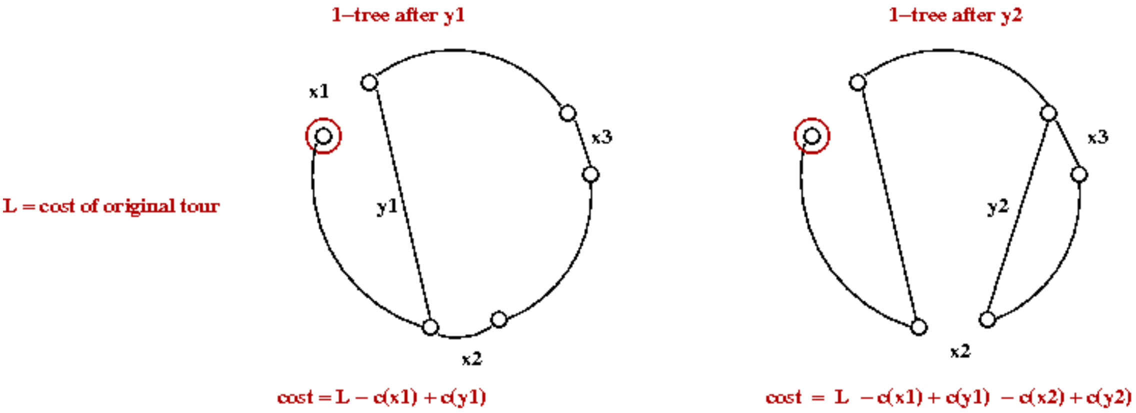
  - Each x_i is an edge in the current tour.
  - Each y_i is NOT in the current tour.
  - They are all unique (no repetitions).
  - The last y_k returns to the starting point t_1

- We'll call this an *LK-move*.

- For example:



- Notice that if we stop at any intermediate y_i, we get a 1-tree.

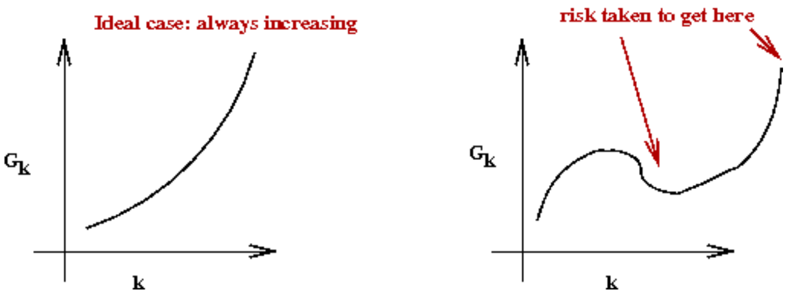


- Let G_1 = gain after first x-y-pair:
  $G_1 = c(x_1) - c(y_1)$

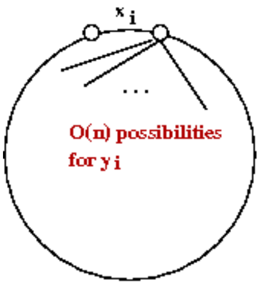
- Similarly,
  $G_2 = c(x_1) - c(y_1) + c(x_2) - c(y_2)$.

- Gain criterion used by algorithm:
  Keep increasing k as long as $G_k > 0$.

- Note: this is a non-trivial addition because it allows for a temporary loss in gain:



- Neighbor limitation:



  - LK limits the number of neighbors to the *m* nearest neighbors, where *m* is an algorithm parameter (e.g., *m=10*).

- Re-starts:
  - Recall: there are *n* choices for t_1, the very first node.
  - LK tries all *n* before giving up.

- Best-tour: at all times LK records the best tour found so far.

- Note: LK is actually a little more complicated than described above, but these are the key ideas.

Performance:

- The standard heuristics (construction, K-OPT) give tours with 2-5% above Held-Karp.

- LK is usually between 1-2% off.

LKH-1: Lin-Kernighan-Helsgaun

From 1999-2009, Keld Helsgaun [Hels2009], added a number of sophisticated optimizations to the basic LK algorithm:

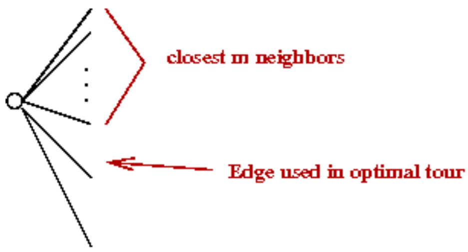
- The first set were added in 1999: [Hels1999].
  → We'll call this LKH-1.
- And the second set in 2009: [Hels2009].
  → We'll call this LKH-2.

Key ideas in LKH-1:

- Use K=5 (prefer this value of K over smaller ones).
  - Experimental evidence showed that the improvement going from 4- to 5-OPT is much better than 3- to 4-OPT.
  - Tradeoff: if K is too high, it takes too long
    → Fewer iterations
    → Less exploration of search space (even if you search a particular neighborhood more thoroughly).

- Relax *sequentiality* allow some x_i's and y_i's to repeat.

- Replace closest *m* neighbors with a different set of *M* neighbors:
  - Problem with LK:



  - Recall best 1-tree in Held-Karp bound?

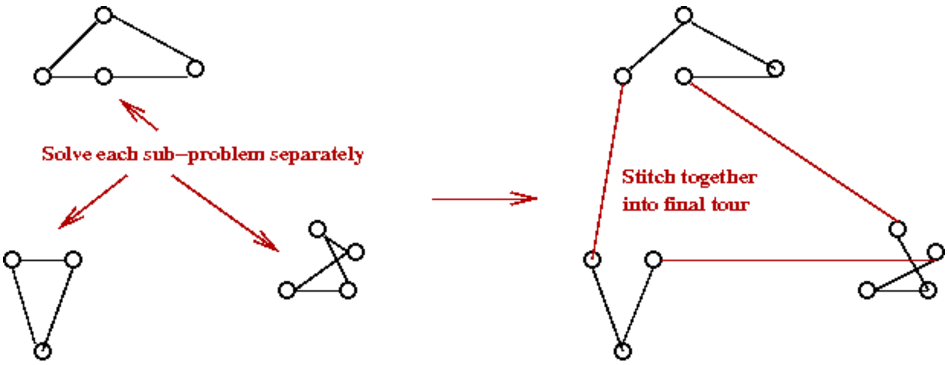
→ Many of these edges are "good" edges for the tour.
→ Experimental evidence: 70-80% of these edges are in optimal tour.

- LKH-1 idea: prefer 1-tree edges that go to neighbors.
- Let $L(T)$ = cost of best 1-tree
  → Can be computed fast (MST)
- For any edge e, let
  $L(T,e)$ = cost of best 1-tree that *must* use e.
- How to force using an edge e?
  - Find min-1-tree.
  - Add e to tree.
  - This causes a cycle.
  - Remove heaviest edge in cycle.
  - This leaves a min-1-tree that uses e.
- Define *&alpha(e)* = $L(T,e)$ - $L(T)$ = importance of e in "1-tree-ness"
- Note: *&alpha(e)=0* for any edge in min-1-tree.
- LKH-1 sorts neighbors by α and uses best m of these.

LKH-2: Lin-Kernighan-Helsgaun, Part 2

Key additions to LKH-1:

- Allow K to increase beyond 5.
- Problem-partitioning:



  - Divide points into clusters.
  - Find best tour for each cluster.
  - Stitch together into final tour.

- Run algorithm many times and merge "best parts" from multiple tours.
  → Called *iterative partial transcription*.
- Use sophisticated tour data structures to speed up running time.
- Results: million city problem with 0.058% of Held-Karp.
  → Within 0.058% of optimal.

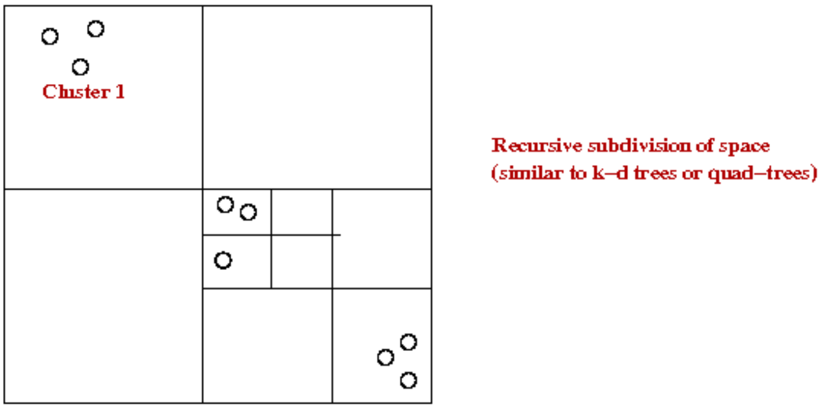
Let's examine the partitioning idea:

- LKH-2 tries a number of partitionings, using different clustering algorithms.
- K-means clustering:

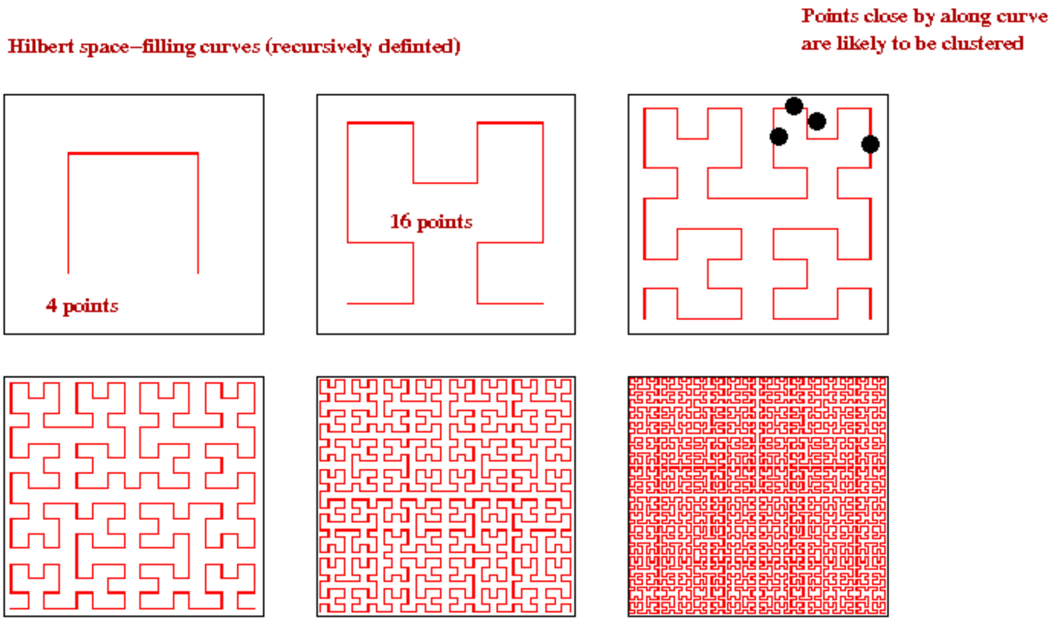
```
1.   repeat
        // Note: this is a different K than in K-OPT.
2.      Pick k centroids.
```

```
3.      Assign each point to closest centroid.
4.      Re-compute the centroid based on assignments.
5.    until no change
```

- Tour segmentation:
  - Run LKH-2 once to find a tour.
  - Segment the tour and re-solve the segments (partition).
- Geometric:

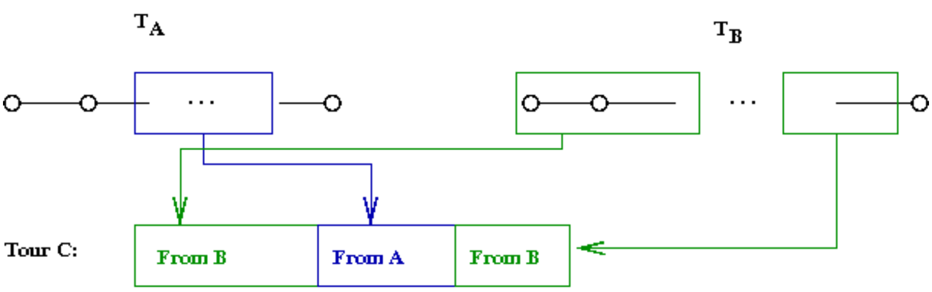


- Space-filling curve:

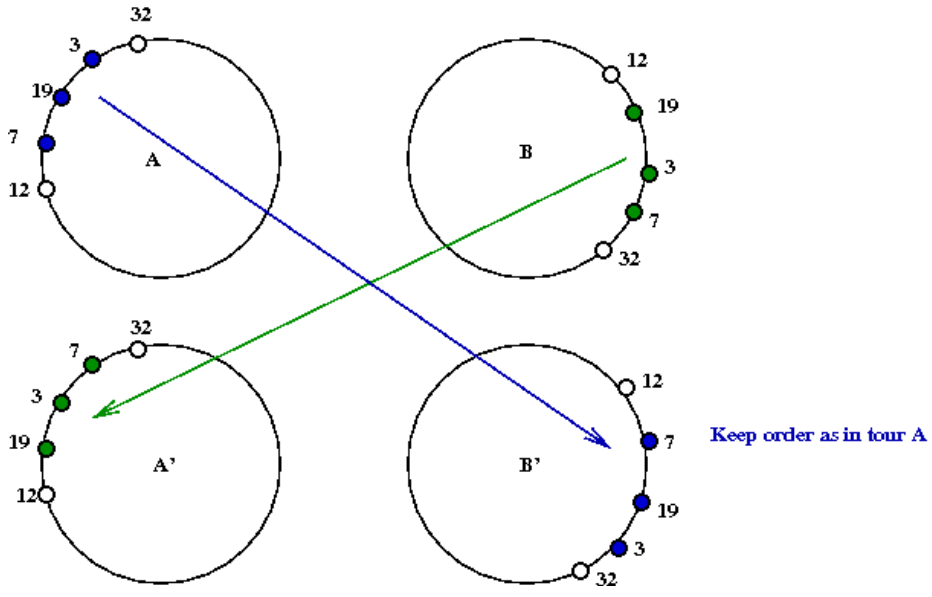


Iterative partial transcription (IPT):

- This is an idea from [Mobi1999].
- Goal: given two tours T_A and T_B, compute T_C that is better than both T_A and T_B.



- A single IPT *trial-swap* between tours T_A and T_B to creates tours $T_{A'}$ and $T_{B'}$



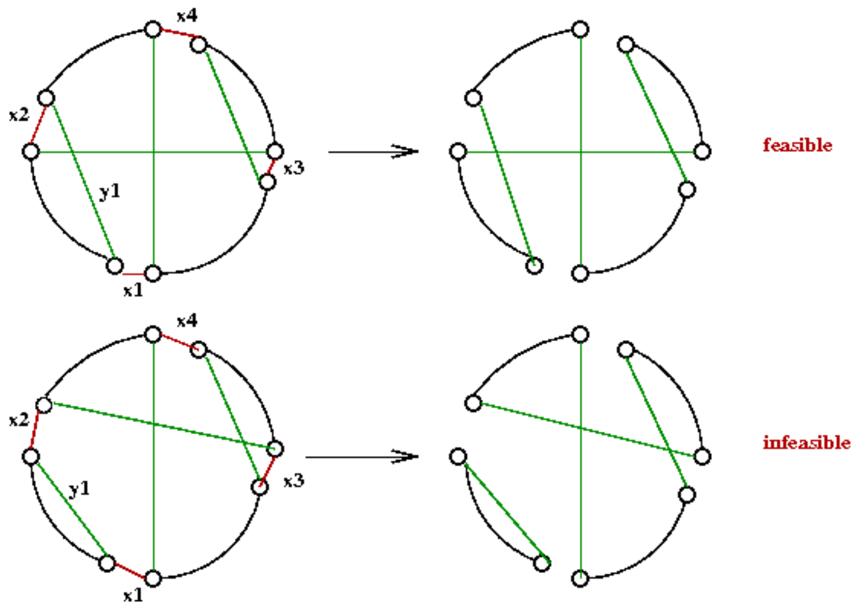
- An IPT-iteration:
  - Identifies all possible valid swap segments.
  - Tries the swaps and identifies the best possible tour that can be generated.

- How to use IPT:
  - Generate *m* tours $T_1, ..., T_m$.
  - For each pair of tours *i,j*, perform an IPT-iteration.

Data structures

Given a K-OPT move, is the resulting "tour" a valid tour?

- Example:

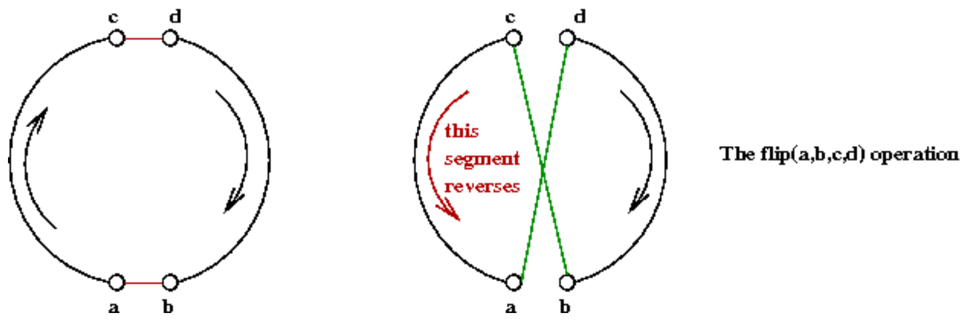


- Naive way: walk along new tour T' to see if all vertices are visited
  → $O(n)$ per trial edge-swap

- Another problem: how to maintain tours?

Operations on tour data structures:

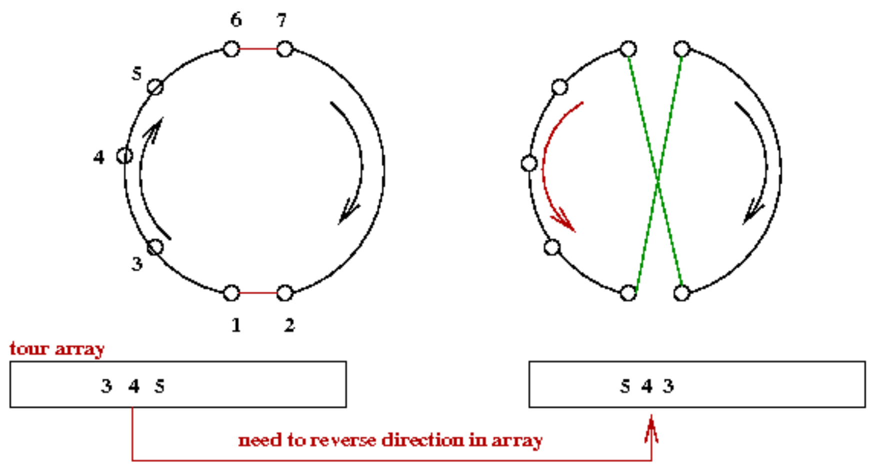
- First, note that any single swap can result in reversing the tour order for one of the segments affected:



- A single 2-OPT move will be called a *flip* operation.
- Also, any K-OPT move can be implemented by a sequence of 2-OPT moves.
  → LK-MOVE can be written to use *flip* operations.
- Other operations that need to be supported:
  - *next(a)*: the next node in tour order.
  - *prev(a)*: the previous node in tour order.
  - *between(a,b,c)*: determine whether *b* is between *a* and *c* in tour-order.
- Note: If a flip is performed correctly, it will result in a valid tour.
- Fredman et al. [Fred1995] show a lower bound of *(log n) / (loglog n)* for these operations.

Arrays:

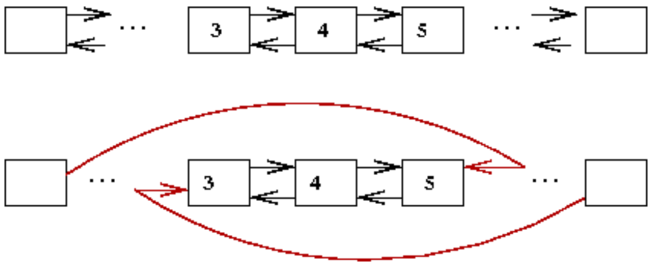
- Simple to implement.
- But consider what needs to be done to reverse a segment:



→ Can take *O(n)*.

Doubly-linked lists:

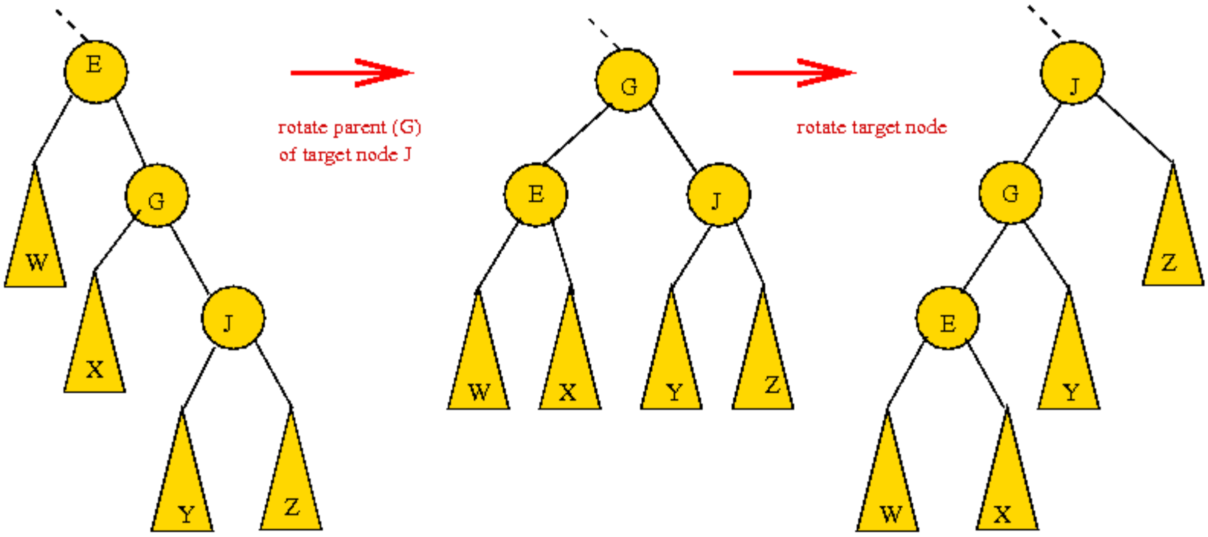
- *flip* takes *O(1)* pointer manipulations.
- Order reversal is also easy (comes for free): *O(1)*.



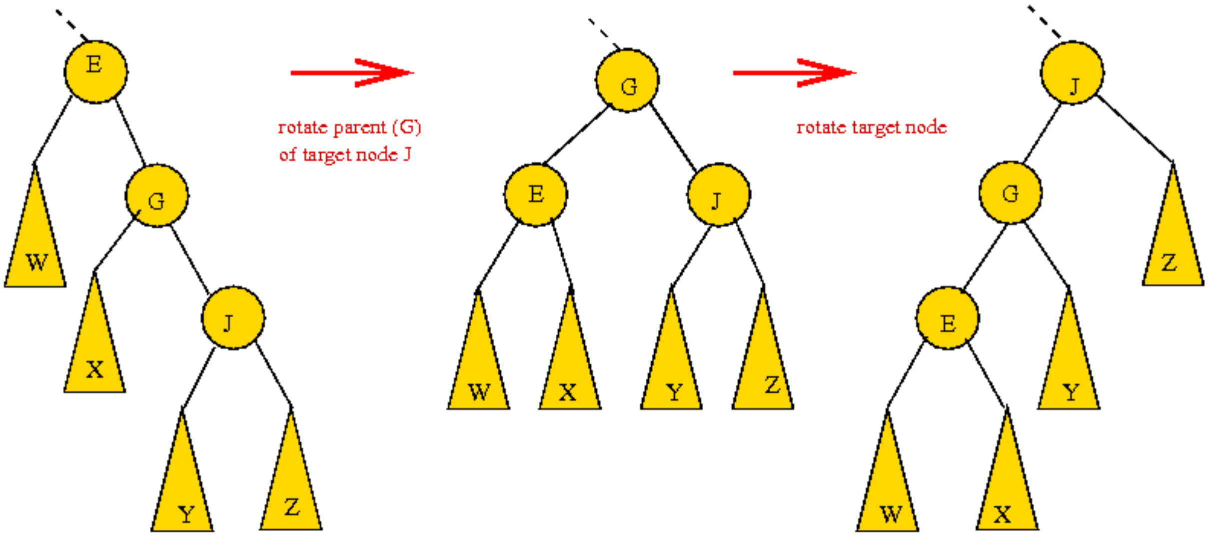
- But finding elements is hard: $O(n)$.

Modified splay trees:

- What is a splay tree?
  - Also called a *self-adjusting binary tree*.
  - See lecture in algorithms course.
  - Recall problem with binary trees: can go out of balance.
  - Problem with forced balance (e.g. AVL): too much overhead.
    → But use of *rotations* is useful.
  - Example of a splay-step: two mini-rotations:

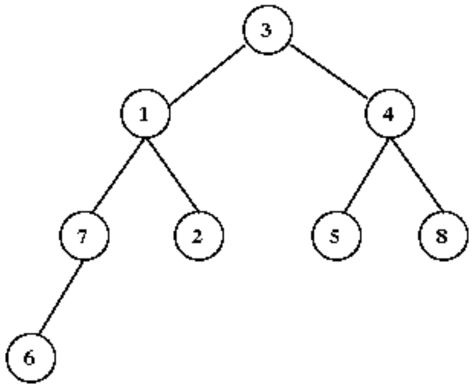


  - Another example:



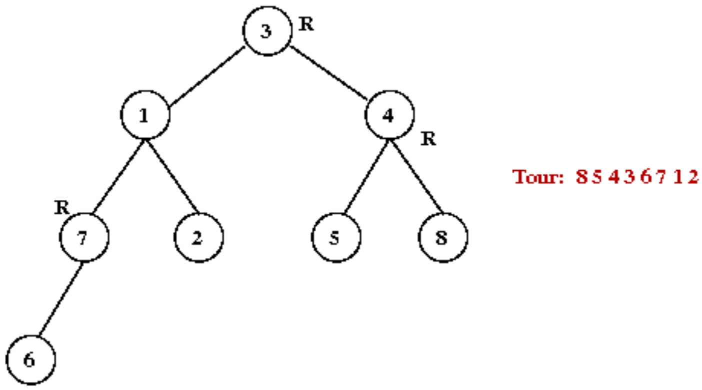
  - In a splay-tree: every accessed node is *splayed to the root*.
    → Similar to Move-to-Front in linked lists.

- Using a splay-tree for a tour:
  - Each node represents a city.
  - Initially, for first tour: in-order traversal is the tour:

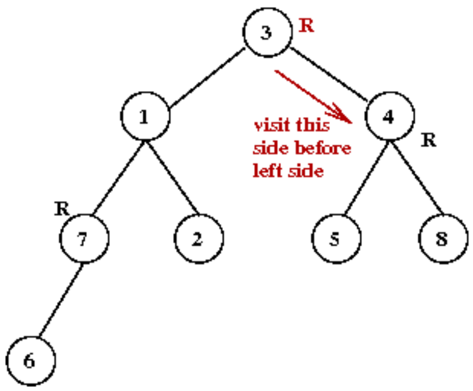


Exercise: What is the tour represented by the above tree?

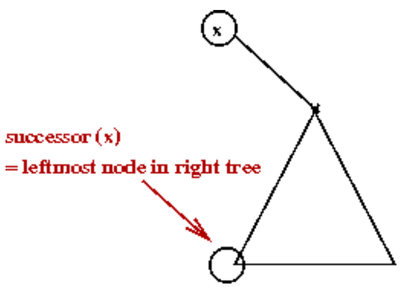
  - Reversals are noted by marking intermediate nodes, e.g.



  - Each time a reversed-node is encountered, switch order (left swapped with right) in in-order traversal:



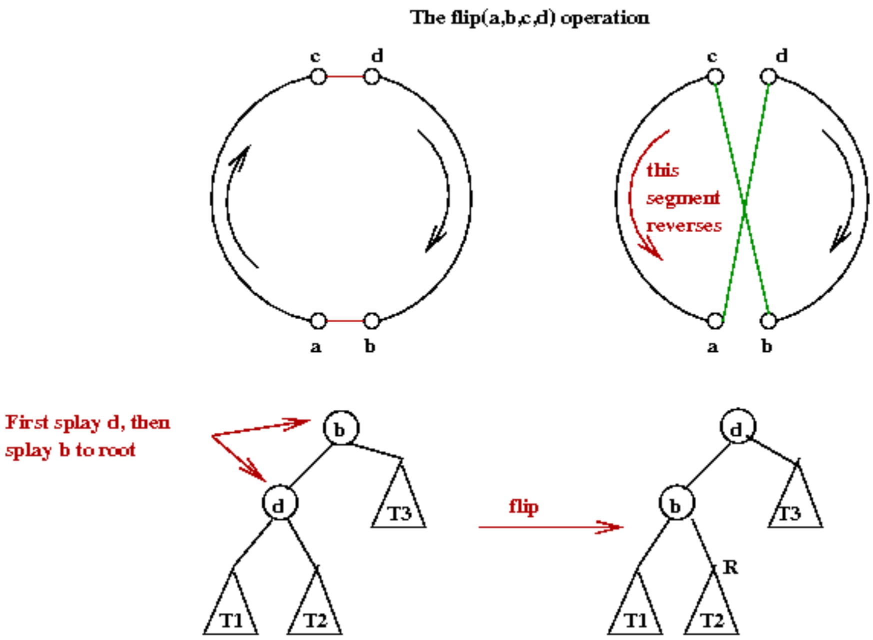
- Maintain an external array of pointers into tree, one per node.
- Implementing *next(a)*:
  - Recall *next(a)* in ordinary binary trees: leftmost node of the right subtree.



  - Locate *a* using pointer-array: *O(1)*.

- Splay to root.
- Find successor using *tour-order* (instead of numeric order).
  → With no reversals, this is the leftmost node of the right subtree.
- With reversals, need to change direction for each flip (when recursing).

- The most complex operation is *flip()*:
  - Just like the splay-tree, there are several different cases.
  - Many involve some type of reversal.
  - The general idea (an example):



The segment tree:

- Devised by Applegate and Cook.

- Based on key observation about LK:
  - You try a sequence of flips (the LK-move).
  - When it doesn't work, you discard the whole sequence.

- In the data structures so far:
  - Every flip changes the data structure.
  - To discard, we need to *undo* flips in reverse order.

- A segment-tree tries to avoid the *undo* part.
  - Array representation of tour.
  - An auxiliary segment-list:
    → To help with tentative flips.
  - An auxiliary segment tree:
    → To help with fast navigation.

Performance:

- Segment-tree is usually best.
- 2-level list is next.
- Splay tree next (with theoretically the best performance).

Exact solution techniques: background

The general idea:

- Formulate TSP as a Integer Programming (IP) problem.
- Apply the *cutting-plane* approach.
- Judicious choice of cutting-plane heuristics.

But, first, what is Integer Programming? We'll need some background in *linear programming*.

Linear programming:

- The word *program* has different meaning than we are used to.
  → More like a "programme" of events.
- An LP (Linear Programming) problem is (in standard form):

$$
\begin{array}{ll}
\max & c_1x_1 + c_2x_2 + \dots + c_nx_n \\
\text{such that} & \\
 & a_{11}x_1 + \dots + a_{1n}x_n \le b_1 \\
 & a_{21}x_1 + \dots + a_{2n}x_n \le b_2 \\
 & \vdots \\
 & a_{n1}x_1 + \dots + a_{nn}x_n \le b_n \\
\text{and} & \\
 & x_i \ge 0, \quad i=1,\dots,n \\
 & x_i \in R
\end{array}
$$

- In vector/matrix notation:

$$
\begin{array}{ll}
\max & c^T x \\
\text{s.t.} & Ax \le b \\
 & x \ge 0
\end{array}
$$

- Example:

3.6 = selling price per unit of product 1

Amount of product 2 = x2

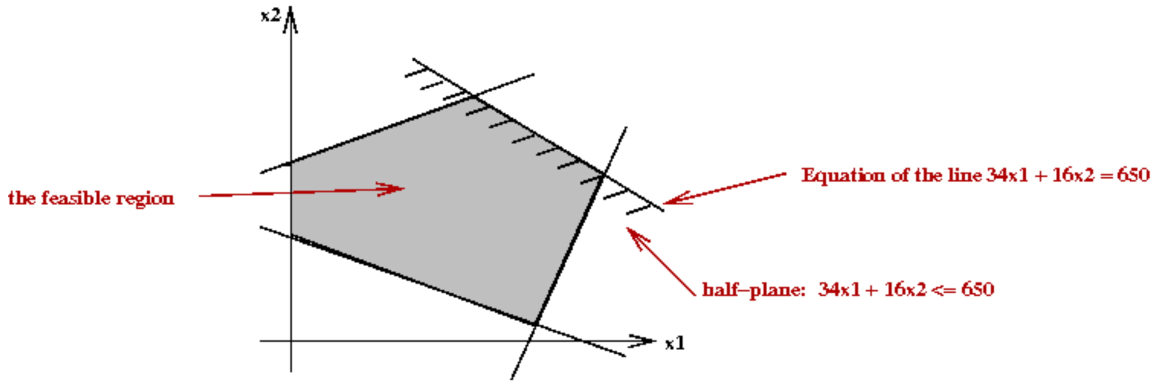
$$
\begin{array}{rrcrcr}
\max & 3.6x_1 & + & 14x_2 & & \\
\text{s.t.} & 12x_1 & + & 23.47x_2 & \le & 400 \\
 & 34x_1 & + & 16x_2 & \le & 650 \\
 & 55x_1 & & & \le & 1200 \\
\text{and} & x_i \ge 0 & & & &
\end{array}
$$

650 = total amount of raw material #2

only product 1 needs raw material #3

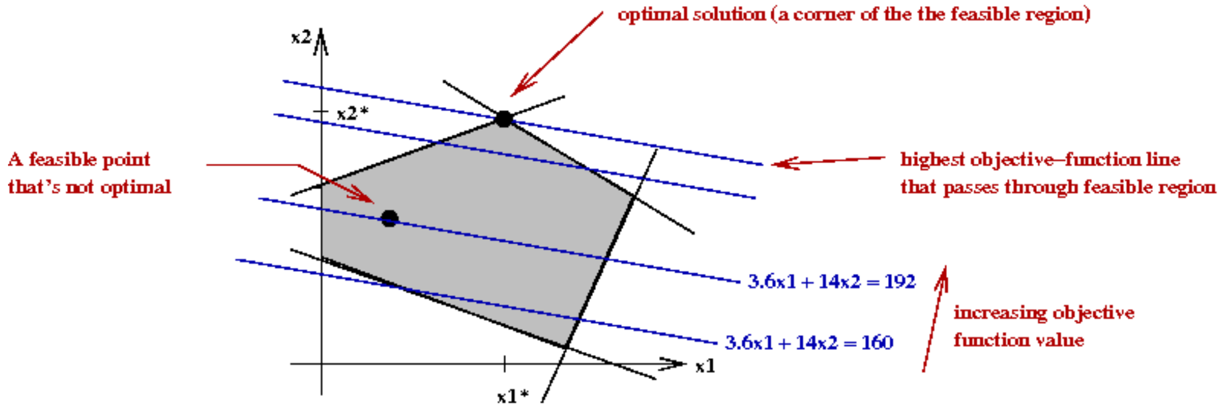
16 = amount of raw material #2 used per unit of product 2

- Geometric intuition of inequality constraints ($Ax \le b$):



- Each inequality defines a half-plane (half-space).
- The intersection is a polytope (polygon in 2D).
- The feasible region is sometimes called the *simplex*.

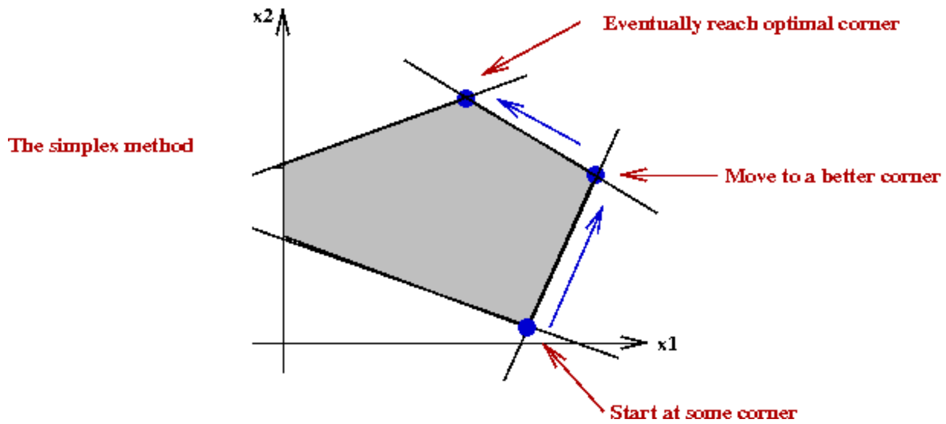
- If we plot objective function "lines":



- If we make a line-equation out of the objective function, some lines will pass through the feasible region.
- Clearly, we want the line with the highest "value" (for a max problem).
- Sweeping the line upwards (higher value), we want the line that is the last line to intersect the feasible region.
- This line always intersects the region at a *corner*.

- Three key algorithms, all major milestones in the development of LP:
  - George Dantzig's Simplex algorithm (1947).
  - Leonid Khachiyan's ellipsoid method (1979).
  - Narendra Karmarkar's interior-point method (1984).

- The simplex method:



- Start at a corner in the feasible region.
- A *simplex-move* is a move to a neighboring corner.
- Pick a better neighbor to move to (or even best neighbor).
- Repeat until you've reached optimal solution.

- What's known about the simplex method:

- Guaranteed to find optimal solution.
- Worst-case running time: exponential.
- In practice, it's quite efficient, approximately $O(n^3)$.
- Very efficient implementations available, both commercial and open-source.
- Has been used to solve very large problems (thousands of variables).

- What's known about the other algorithms:
  - Khachiyan's ellipsoid method: provably polynomial, but inefficient in practice.
  - Karmarkar's algorithm: provably polynomial and practically efficient for many types of LP problems.

- Note: an LP problem with equality constraints

```
max    cTx
s.t.   Ax = b
        x ≥ 0
```

can be converted to an equivalent one in standard form (with inequality constraints).

- Similarly, a min-problem can be convertex to a max-problem.

Integer programming:

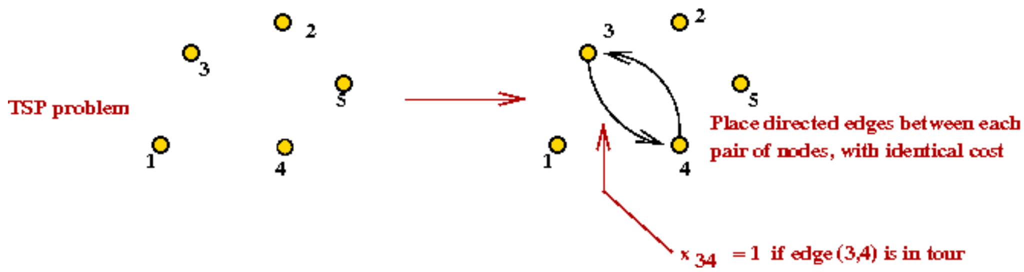
- An integer program (IP) is an LP problem with one additional constraint: all x_i's are required to be integer:

```
max    cTx
s.t.   Ax ≤ b
        x ≥ 0
        x ε Z
```

Exact solution techniques: TSP as an IP problem

First, let's express TSP as an IP problem:

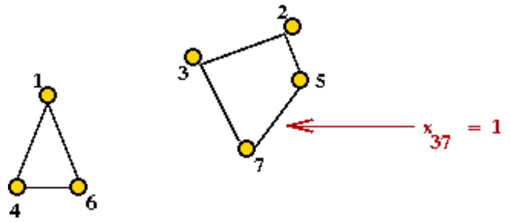
- We'll assume the TSP is a Euclidean TSP (the formulation for a graph-TSP is similar).
- Let the variable x_{ij} represent the directed edge (i,j).
- Let $c_{ij} = c_{ji}$ = the cost of the undirected edge (i,j).



- Consider the following IP problem:

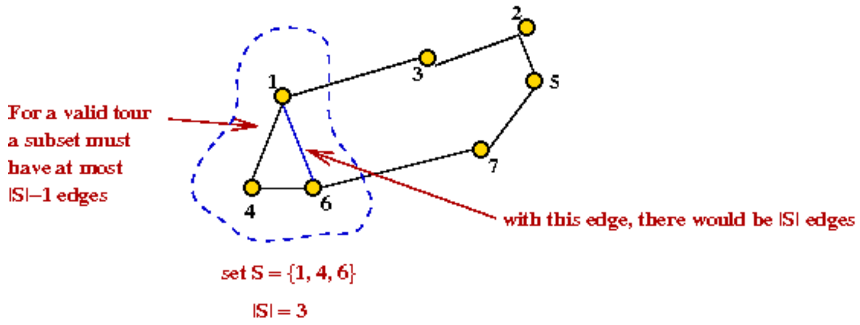
```
min     Σi,j  ci,j xi,j
s.t.     Σj xi,j = 1          // Only one outgoing arc from i
         Σi xi,j = 1          // Only one incoming arc at j
```

- Unfortunately, this is not sufficient:



You can get multiple cycles.
→ Called *sub-tours*

- What to do? Consider this idea:



  - Consider a subset of vertices S.
  - In a valid tour,
    $\Sigma_{i,j}\, x_{i,j} \leq |S|-1$ for all $i,j\ \varepsilon\ S$.
  - This is an inequality constraint that could be added to the IP problem.
    → Called a *sub-tour* constraint.

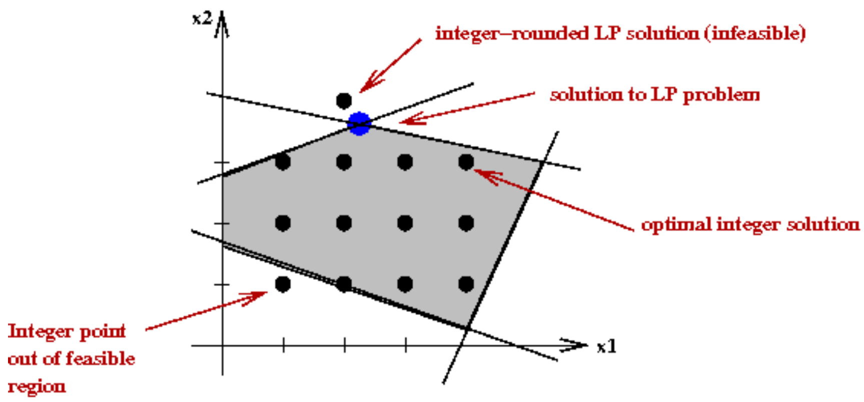
- How many such constraints need to be added to the IP problem?
  → One for each possible subset S.
  → Exponential number of constraints!

- Fortunately, one can add these constraints only as and when needed (see below).

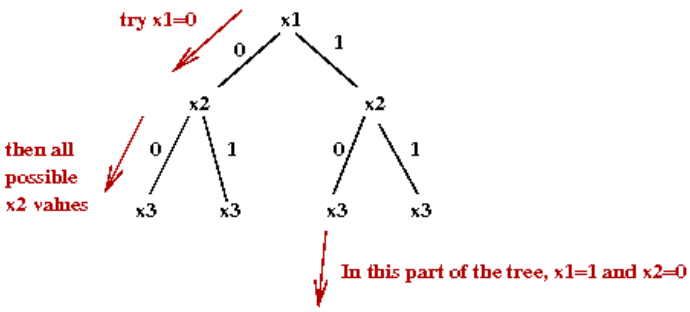
Solving the IP problem:

- Naive approach:
  - Solve the *LP relaxation* problem first.
    → Remove integer constraints (temporarily) to get a regular LP, and solve it.
  - Round LP solution to nearest integers.

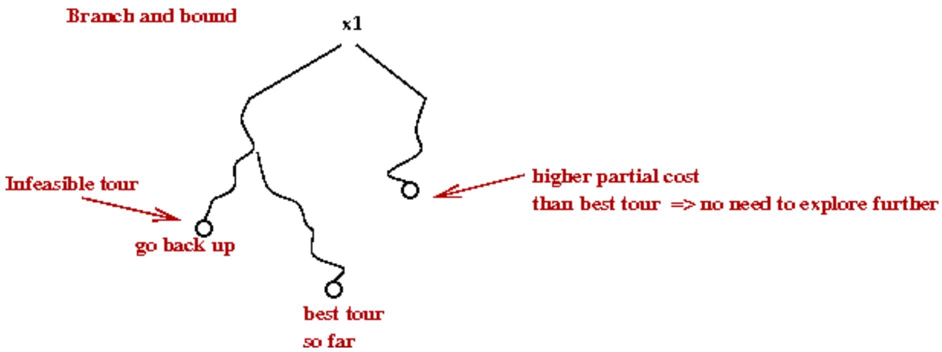
  Unfortunately, this may not yield a feasible solution:



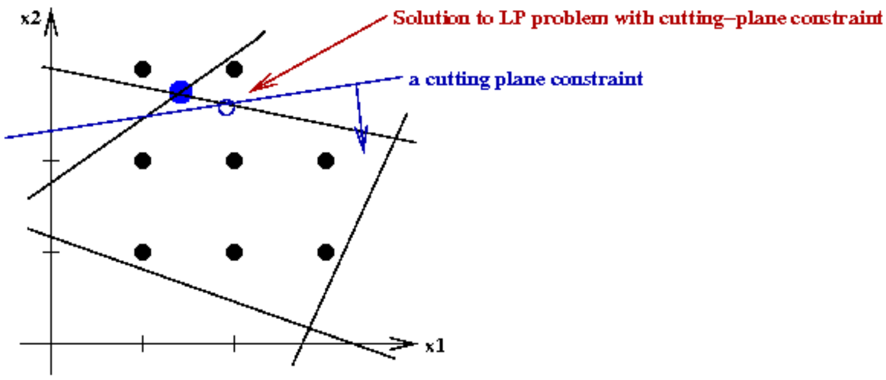
- Branch-and-bound:
  - We'll explain this for 0-1-IP problems (variables are binary-valued).
  - First, consider a simple exhaustive search, organized as a tree-search (the "branch" part):



- The tree itself can be explored in a variety of ways:
  - Breadth-first (high me
    → High memory requirements.
  - Depth-first
    → Low memory requirements.
  - Cost-first
    → Expand the node that adds the least overall cost to the (partial) objective function.
- Note: if the cost to a node already exceeds the best tour so far, there's no need to explore further.
  → Parts of the tree can be *pruned*.



- Cutting planes:



  - Add constraints to force the LP-solutions towards integers.
  - With a sequence of such constraints, such a process can converge to an integer solution.
  - However, it can take a long time.

- Gomory's algorithm:
  - A general cutting-plane algorithm for any IP.
  - The idea:
    - Solve LP.
    - Examine equations satisfied at corner point (of LP).
    - Round to integers in inequalities involving those variables.
    - Add these to constraints.
    - Repeat.
  - Unfortunately, it is slow in practice.

History of applying IP to TSP:

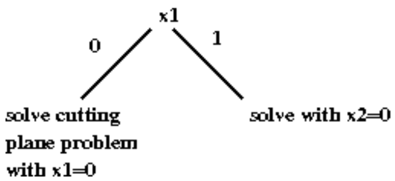
- Original cutting plane idea due to Dantzig, Fulkerson and Johnson in 1954.
    - Idea:

```
repeat
    solve LP
    identify sub-tours (cycles) and add corresponding "|S|-1" constraints.
until full-tour found
```

    - Dantzig et al added a few more "sub-tour" like constraints.

- Today, there are several families of cutting-plane constraints for the TSP.

- Branch-and-cut
    - Cutting planes "ruled" until 1972.
    - Saman Hong (JHU) in 1972 combined cutting-planes with branch-and-bound
      → Called branch-and-cut.
    - The idea: some variables might change too slowly with cutting planes
      → For these, try both 0 and 1 (branch-and-bound idea).
    - Alternate way of viewing this:



- More sophisticated "cut" families:
    - Grotschel & Padberg, 1970's.
    - Padberg and Hong, 1980: 318-city problem.
    - Grotschel and Holland, 1987: 666-city problem.
    - Padberg and Rinaldi, 1987-88: combined multiple types of cuts, branch-and-cut and various tricks to solve 2392-city problem.

- During this time, LP techniques improved greatly
  → Can cut down "active" variables in an LP problem.

- Applegate et al (2006)
    - Sophisticated LP techniques, new data structures.
    - 85,900 city problem.

References and further reading

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Note: The Hilbert curve was an image found on Wiki-commons.