

Traveling Salesman Problem (TSP): Foundations and Methods

The **Traveling Salesman Problem (TSP)** asks: "Given a list of cities and the distances between each pair, what is the shortest possible route that visits each city exactly once and returns to the origin?" 1. In graph-theoretic terms, TSP is modeled on a **complete weighted graph**: cities are vertices, edges are possible paths with weights equal to distances or costs, and a *tour* is a Hamiltonian cycle (visiting each vertex once and returning to start) of minimal total weight 2 3. (If distances differ by direction, one has the *asymmetric TSP* on a directed graph 4.)

TSP is **computationally intractable** in general. The decision version ("is there a tour of length \leq L?") is **NP-complete**, and the optimization version is **NP-hard** ¹ ⁵ . This means no polynomial-time algorithm is known, and the worst-case running time grows *superpolynomially* (e.g. factorial or exponential) with the number of cities ⁶ ⁵ . For example, the naive brute-force search tries all n! tours, an astronomical number for even moderate n. In fact, a modern analysis shows brute force takes $\Theta(n!)$ time, whereas the dynamic-programming Held–Karp algorithm runs in $\Theta(2^n n^2)$ time ⁷ – an exponential improvement but still only practical for n in the tens. (Held–Karp DP uses bitmasks to represent subsets and exactly solves TSP in exponential time ⁸ ⁷ .)

Because of this complexity, TSP is a benchmark for optimization and algorithm research ⁹. State-of-the-art solvers (e.g. Concorde) have used cutting-plane (branch-and-cut) methods to solve instances up to tens of thousands of cities exactly. For example, Grötschel, Padberg et al. solved a 2,392-city instance using cutting planes and branch-and-bound ¹⁰, and Concorde later solved a famous 85,900-city "chip layout" problem ¹¹. For even larger instances (millions of points), one can find tours guaranteed within a few percent of optimal ¹¹.

Exact Solution Methods

- **Brute Force.** Check all permutations of cities (n! tours). Guaranteed to find the optimal tour, but only feasible for tiny n. Time grows *super-exponentially* ($\Theta(n!)$) 7 .
- **Dynamic Programming (Held–Karp).** Uses DP over subsets of cities to compute shortest paths that visit each subset. Runs in $\Theta(2^n n^2)$ time and uses $\Theta(n 2^n)$ memory 7. It finds the exact optimum for n up to $\sim 20-30$ in reasonable time.
- **Branch and Bound / Branch and Cut.** Systematically build tours by extending partial routes ("branch") while pruning any branch whose partial cost plus a lower-bound estimate already exceeds the best known solution. Lower bounds come from relaxations (e.g. minimum 1-tree or assignment problem). Modern implementations combine B&B with cutting-plane methods (branch-and-cut) to eliminate fractional subtours in an integer program. This approach powers solvers like Concorde, which have solved very large instances to optimality 10 11.

Approximate and Heuristic Methods

Because exact algorithms scale poorly, many **heuristics** and **metaheuristics** are used in practice. These aim to find *good* (not always optimal) tours quickly:

- Nearest Neighbor. Start at a random city, then repeatedly go to the nearest unvisited city 12. This greedy method is extremely fast (O(n^2) time) but can miss the optimal tour by a large factor 12. It often yields a quick initial solution for further improvement.
- **Greedy Insertion (e.g. cheapest insertion).** Build a tour by repeatedly inserting the city that causes the least increase in cost. Variants include nearest insertion and farthest insertion. These are simple constructive heuristics that run in polynomial time.
- Christofides' Algorithm (Metric TSP). For metric (satisfying triangle inequality) symmetric TSP, Christofides' algorithm is a famous 3/2-approximation: it guarantees the tour length ≤1.5×optimal ¹³. It works by building a minimum spanning tree, finding a minimum-weight perfect matching on odd-degree vertices, and combining to form an Eulerian graph from which a tour is extracted. This polynomial-time approximation is often used when optimality can be slightly relaxed ¹³.
- 2-opt, 3-opt and k-opt Local Search. Starting from any tour, repeatedly improve it by local swaps: e.g. 2-opt removes two edges and reconnects the tour in the best alternative way without crossings. Lin–Kernighan (LKH) is a powerful variable-k local search that adaptively chooses sequences of swaps. These "opt" heuristics are very effective in practice and are often used to refine tours from other heuristics.
- **Genetic Algorithms (GA).** Treat each tour as a "chromosome." Start with a population of random tours, then iteratively apply selection (favor shorter tours), crossover (combine parts of two tours), and mutation (randomly swap edges) ¹⁴. GAs explore diverse solutions and can escape local optima via randomness. They do not guarantee optimality, but can find good tours for moderate sizes. (Implementation details vary, e.g. order crossover, partially matched crossover, etc.)
- **Simulated Annealing.** A physics-inspired metaheuristic. Start with a tour and a "temperature" parameter. Make random small changes (e.g. 2-opt swaps): if the new tour is shorter, always accept it; if longer, accept it with a probability that decreases with the temperature ¹⁵. Initially, at high temperature, the algorithm is more likely to accept uphill moves, allowing escape from local minima; then the temperature "cools" and the search focuses on fine improvements. Over time this yields a near-optimal tour. In summary: "when the temperature is high, larger random changes are made (avoiding local minima), then homing in on a near-optimal minimum as the temperature falls" ¹⁵.
- Ant Colony Optimization (ACO). A population-based metaheuristic inspired by foraging ants ¹⁶. Artificial "ants" build tours probabilistically: they deposit virtual "pheromone" on edges they traverse, biased by shorter-path success. Edges with more pheromone are more likely to be chosen by future ants, reinforcing good routes. Iteratively, pheromones evaporate and are renewed so that the colony converges on a high-quality path ¹⁶. ACO is especially popular for routing problems and has been applied to large TSP instances.

• **Particle Swarm Optimization (PSO).** Originally for continuous optimization, PSO can be adapted to discrete TSP. In PSO, each "particle" represents a candidate tour (often encoded as a permutation). Particles move in the solution space influenced by their own best-known solution and the swarm's global best ¹⁷. Over iterations, particles "fly" towards good solutions. In effect, PSO is a metaheuristic where solutions are guided by collective learning, and has shown promise on TSP variants.

These heuristics trade optimality for speed and scalability. In practice, one often combines them: e.g., start with a greedy or GA-generated tour, then apply 2-opt or LKH to polish it. For metric TSP, Christofides' algorithm remains a theoretical benchmark (1.5-approx) ¹³, though in practice LKH often finds optimal or near-optimal tours on random Euclidean data.

Convex-Optimization Relaxations

Though TSP is combinatorial, one can apply convex optimization ideas via **relaxations**. A common approach is to formulate TSP as an integer linear program (ILP). For example, in the standard formulation each directed edge has a binary variable indicating if it's in the tour, and subtour-elimination constraints enforce a single cycle. Dropping the integrality yields an LP (a convex program) that can be solved efficiently. The optimal value of this **LP relaxation** is a *lower bound* on the true tour length. Notably, the Held-Karp bound is essentially the optimum of a special LP relaxation. This is used, for instance, in branch-and-cut: one solves the relaxed LP, adds violated subtour cuts, and iterates towards integrality. (See the Held-Karp formulation which "relaxes" the integer program so variables can be continuous, yielding a lower bound ¹⁸.)

More sophisticated convex methods (e.g. semidefinite-programming relaxations) have been studied to tighten the bound, but they are complex and rarely used in practice. The main takeaway is that convex relaxation provides a way to prune search (via strong lower bounds) but by itself yields fractional solutions. Complete solutions require further branching or cutting planes.

Real-World Applications

TSP and its variants arise in numerous domains:

- **Logistics and Routing:** The classic application is planning delivery or inspection routes. For example, a salesperson or delivery truck wants the shortest tour visiting customers (TSP). In real companies, multiple vehicles or depots are involved, leading to the *Vehicle Routing Problem (VRP)*19, a generalization of TSP. (Google's OR-Tools, for instance, provides VRP solvers with capacity and time-window constraints.) Optimization of routes can save 5–30% in travel costs
 20.
- Manufacturing and Circuit Design: In PCB drilling or milling, a machine (robot) must visit many holes or parts. Scheduling the drill path to minimize non-cutting moves is a TSP ²¹. Similarly, in the fabrication of microchips or printed circuit boards, tools (e.g. for soldering or inspection) follow TSP tours. For example: "A classic example is in printed circuit manufacturing: scheduling the route of the drill machine to drill holes in a PCB. In robotic machining/drilling, the 'cities' are holes to drill, and the 'cost' includes time for retooling the robot." ²¹.
- **Astronomy:** Observatories schedule telescopes to observe many targets (stars, galaxies). TSP arises by modeling each target as a "city" and slewing time between targets as distance. Minimizing total repositioning time leads to a TSP embedded in a larger control problem 22. This can dramatically increase observing efficiency.

- **Robotics and Automation:** A mobile robot or automated guided vehicle (AGV) often must visit a set of waypoints or perform tasks in different locations. Path planning to cover all points with minimal travel (a "lawnmower" or inspection robot) is a TSP variant. The TSP-with-service (where each "customer" has a service time) and TSP-with-time-windows (each waypoint must be reached within a time window) are common in scheduling mobile robots.
- **Genomics and Bioinformatics:** TSP-like formulations appear in DNA sequencing and protein/ ligand design. For instance, in DNA fragment assembly, one seeks a path through fragments minimizing overlaps; cities represent fragments, and distances are inverse overlaps ²².
- Other Areas: Planning tourism or garbage collection routes, fiber-optic or cable routing, and data routing in networks all can involve solving a TSP. In each case, a "city" can represent anything (customer, drill-hole, gene fragment) and "distance" can be cost, time, or inverse similarity 22.

In many of these applications, additional constraints modify the TSP: e.g., time windows (deliver by a certain time), vehicle capacities (VRP), or precedence/order requirements. These lead to well-studied variants like the *TSP with Time Windows (TSPTW)*, the *Prize-Collecting TSP*, and the *Generalized TSP (clusters of cities)*, among others ²³. The VRP is perhaps the most prominent generalization, asking for optimal multi-vehicle routes ¹⁹.

Variations and Related Problems

TSP's rich structure has inspired many extensions and related models:

- Multiple Salesmen (mTSP) / Vehicle Routing (VRP). More than one salesman or vehicle is allowed. The goal may be to cover all cities using multiple tours, often minimizing total cost or balancing loads. The VRP (a classical logistics problem) generalizes TSP by including multiple vehicles, depots, and capacity/time-window constraints 19 24.
- **Time Windows:** Each city must be visited within a specified time interval. The *TSP with Time Windows (TSPTW)* adds scheduling constraints to the tour. For example, delivery locations might only be accessible between certain hours. VRP solvers often include time-window features.
- Asymmetric TSP (ATSP): Distances are not symmetric ($d(i,j) \neq d(j,i)$), such as with one-way streets or different flight costs. ATSP can be reduced to symmetric TSP by doubling cities, but specialized algorithms exist. Many heuristics (NN, SA, ACO) apply equally to ATSP.
- **Generalized TSP:** Cities are partitioned into clusters (or "cities and states"), and the salesman must visit exactly one city in each cluster ²³. This arises in problems like drilling (choose one hole from each slot), or sales calls (visit one representative in each region).
- **Bottleneck TSP:** Minimize the maximum edge length used, rather than total length. For example, scheduling a drill to avoid long moves or heavy loads. This is important in avoiding worst-case delays 21.
- Other variants: Many more have been studied, including open TSP (no return to start), mileage TSP (minimize sum of squares of distances), probabilistic TSP (cities appear with probability), etc. Each arises from practical tweaks to the basic assumptions.

• **Related Graph Problems:** TSP is closely related to the Hamiltonian cycle problem (does *any* tour exist?), and to shortest-path trees, spanning trees, and matching problems (used in heuristics like Christofides). Techniques developed for TSP often translate to these areas.

Overall, **TSP** is a cornerstone of combinatorial optimization. It has driven advances in integer programming, cutting-plane methods, and metaheuristic design. For example, the celebrated *Lin-Kernighan heuristic* (a sophisticated k-opt) and *Concorde* solver (branch-and-cut with cutting planes) were developed with TSP in mind. TSP solutions also provide benchmarks: the TSPLIB instance library has dozens of real and random test cases that researchers use to compare algorithms. Solvers like Concorde have tackled TSPLIB instances with up to ~85,900 cities optimally ¹¹.

Resources and Tools

For hands-on exploration, there are many code libraries and visual tools:

- Python and Libraries:
- **NetworkX:** Includes a traveling_salesman_problem function with several heuristics (Christofides, greedy, simulated annealing, etc.) ²⁵. For example, nx.algorithms.approximation.traveling_salesman.traveling_salesman_problem can solve or approximate small TSPs.
- OR-Tools (Google): The OR-Tools suite provides routing solvers that handle TSP/VRP with
 constraints. Its documentation and examples (e.g. <u>Vehicle Routing guides</u>) show how to model
 and solve TSP, VRP, and variants with time windows, capacities, etc.
- **Python Libraries and Code:** There are dedicated packages (e.g. python-tsp on PyPI) and many GitHub repositories with example implementations. For instance, <u>jacobcwright/TSP-python</u> demonstrates basic TSP algorithms. Visualization projects like <u>pyTSP</u> let you see 2D/3D tours and heuristics in action.
- · C/C++ Solvers:
- **Concorde:** A state-of-the-art exact TSP solver (written in C). It can be downloaded from the authors' site (University of Waterloo) and includes tools for TSPLIB formats.
- **LKH (Lin–Kernighan Heuristic):** An advanced C implementation of Lin–Kernighan for very large TSP instances.
- **Web/Visual Tools:** Online applets and interactive demos exist for learning TSP: e.g. web-based visualizations of 2-opt swaps or ant-colony behaviors. (One example is the Fourmilab TSP demonstration for simulated annealing 15 .)
- **Benchmark Instances (TSPLIB):** The <u>TSPLIB</u> is a library of sample TSP (and related) instances from real and random data. It is widely used for testing algorithms.
- **Tutorials and Courses:** Many textbooks and online courses cover TSP. Useful links include GeeksforGeeks and educational blogs on implementing GA/SA for TSP. For example, the GeeksforGeeks page on TSP with genetic algorithms ¹⁴ provides code snippets.

These resources offer code examples and allow experimentation with the TSP and its variants. They make the problem accessible to beginners while also supporting advanced research and large-scale computations.

Sources: Authoritative sources include Wikipedia and academic literature on TSP $\begin{smallmatrix}1&&2&15&16&17\end{smallmatrix}$ $\begin{smallmatrix}13&&21\end{smallmatrix}$, as well as solver documentation and optimization guides $\begin{smallmatrix}19&&25\end{smallmatrix}$, from which key concepts and algorithms have been drawn.

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