CS498: Algorithmic Engineering

Lecture 16: Non-Convex Landscapes, Simulated Annealing & Genetic Algorithms

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Outline

Where We Are in the Course

Part I (Lectures 1–9):

- LP, IP, modeling patterns.
- Branch-and-bound.
- Row generation, lazy cuts.
- **Philosophy:** structured discrete problems $\Rightarrow$ exact solvers.

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Part II (Lectures 10–15):

- Gradient descent, PyTorch.
- Projected GD, penalty methods.
- Lagrangian duality, KKT, SDP.
- **Philosophy:** convexity $\Rightarrow$ every local min is global.

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Today (last lecture in Part II): What do we do when *neither* assumption holds?

We will revisit gradient descent/ML after part III of the course (SAT/SMT Solvers).

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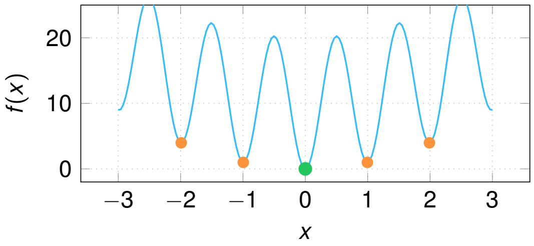

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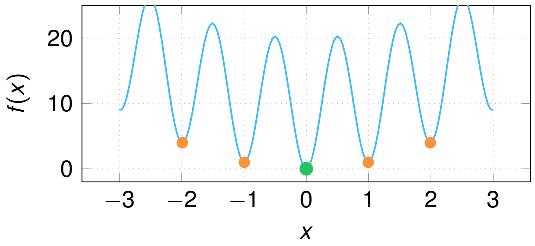

This is the **Rastrigin function**. Global minimum at $x = 0$, but local minima *everywhere*. Gradient descent converges to whichever local minimum is nearest to the starting point.

GD Gets Stuck: A Concrete Demonstration

```python
import torch

def rastrigin(x):
    return x**2 - 10 * torch.cos(2 * torch.pi * x) + 10

x = torch.tensor(1.7, requires_grad=True)    # start near a local min
alpha = 0.01
for k in range(500):
    loss = rastrigin(x)
    loss.backward()
    with torch.no_grad():
        x -= alpha * x.grad
        x.grad.zero_()

print(f"x = {x.item():.4f}, f(x) = {rastrigin(x).item():.4f}")
# x = 1.8203,  f(x) = 9.0374    <-- stuck at a local minimum!
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Random restarts help, but in d dimensions with m local minima per axis, there are m^d local minima total. You cannot restart your way out.

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For now: when the problem is low-dimensional, combinatorial, or has no usable gradients at all, GD is not an option. That's where metaheuristics come in.

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The gap

GD needs convexity (or gradients). B&B needs structure and moderate size.
What if we have neither?

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This leads us to **Simulated Annealing**.

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Optimization analogy:

- "Energy" = objective $f(x)$.
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- "Temperature" T = willingness to accept bad moves.

- High T: explore broadly.
- Low T: refine locally.
- Slowly decrease $T \to 0$.

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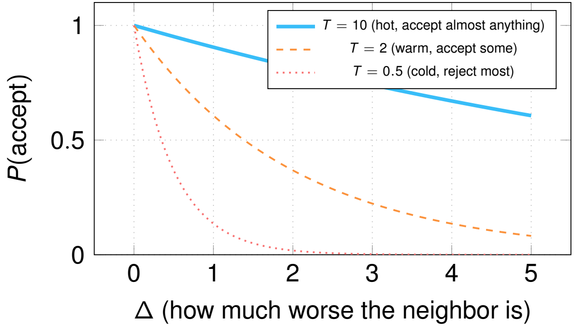
In words: small worsenings are accepted often; large worsenings are accepted rarely. At high temperature, almost everything is accepted. At low temperature, almost nothing bad is accepted.

Metropolis Criterion: The Picture



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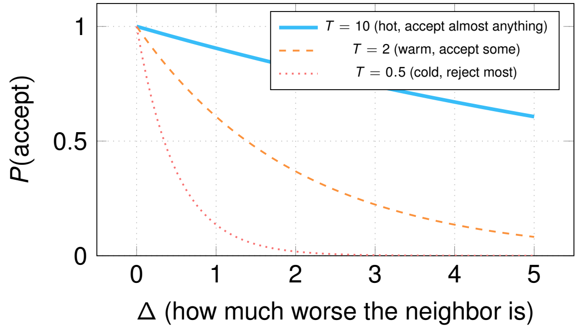

As $T \to 0$, SA behaves like greedy descent. As $T \to \infty$, SA behaves like random walk.

The SA Algorithm

Simulated Annealing

1. Start with an initial solution x and temperature T_0.
2. **Repeat** for $k = 1, 2, \ldots$:
    1. Generate a random **neighbor** x' of x.
    2. Compute $\Delta = f(x') - f(x)$.
    3. If $\Delta < 0$: accept ($x \leftarrow x'$).
    4. Else: accept ($x \leftarrow x'$) with probability $e^{-\Delta/T}$.
    5. Decrease temperature: $T \leftarrow \alpha \cdot T \quad$ (for example $\alpha \approx 0.9995$).
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That's it. The entire algorithm fits in 10 lines of code.

Temperature Schedules

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Geometric cooling (practical):

$$T(k) = T_0 \cdot \alpha^k$$

Typical: $\alpha \in [0.99, 0.9999]$.

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Provably converges to the global optimum (Hajek, 1988).

But: logarithmic cooling is *so slow* it is essentially brute-force enumeration. Nobody uses it.

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Takeaway: use geometric cooling with $\alpha \approx 0.995$, tuned by trial and error. Run multiple independent restarts. No guarantees, but excellent results in practice.

SA on Rastrigin: The Fix

Recall: GD got stuck at a local minima. Let’s try SA on the same function.

```
import numpy as np

x = 1.7                         # same starting point as GD
best_x, best_f = x, x**2 - 10*np.cos(2*np.pi*x) + 10
T = 10.0

for k in range(200_000):
    x_new = x + np.random.randn() * 0.5          # random neighbor
    f_old = x**2 - 10*np.cos(2*np.pi*x) + 10
    f_new = x_new**2 - 10*np.cos(2*np.pi*x_new) + 10
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    if delta < 0 or np.random.random() < np.exp(-delta / T):  # Metropolis
        x = x_new
    if f_new < best_f:
        best_x, best_f = x_new, f_new
    T *= 0.99997                                  # geometric cooling

print(f"x = {best_x:.4f}, f(x) = {best_f:.4f}")
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Same starting point, but SA escaped the local minimum that trapped GD.

TSP: From ILP to Permutations

In Lectures 7 and 9, we modeled TSP as an **integer linear program**:

- Binary arc variables $x_{ij} \in \{0, 1\}$.
- Degree constraints: each city has exactly one incoming and one outgoing arc.
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No ILP. No Gurobi. No subtour constraints. Every permutation is automatically a valid tour.

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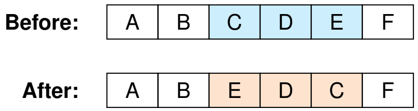

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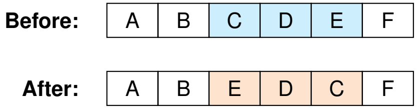

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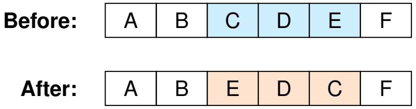

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Key observation: It is the most widely used neighborhood for TSP.

An alternative is **swap**: exchange the positions of two random cities. Simpler, but less effective.

SA for TSP: Full Implementation

```python
import numpy as np

def tsp_sa(dist, T0=100.0, alpha=0.9995, n_iter=500_000):
    n = len(dist)
    tour = list(range(n))
    np.random.shuffle(tour)
    cost = sum(dist[tour[i]][tour[(i+1) % n]] for i in range(n))
    best_tour, best_cost = tour[:], cost
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    for k in range(n_iter):
        i, j = sorted(np.random.randint(0, n, size=2))  # 2-opt: pick segment
        if i == j: continue
        new_tour = tour[:i] + tour[i:j+1][::-1] + tour[j+1:]  # reverse it
        new_cost = sum(dist[new_tour[a]][new_tour[(a+1)%n]] for a in range(n))
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        delta = new_cost - cost
        if delta < 0 or np.random.random() < np.exp(-delta / T):   # Metropolis
            tour, cost = new_tour, new_cost
            if cost < best_cost:
                best_tour, best_cost = tour[:], cost
        T *= alpha
    return best_tour, best_cost
```

SA for TSP: Full Implementation

```python
import numpy as np

def tsp_sa(dist, T0=100.0, alpha=0.9995, n_iter=500_000):
    n = len(dist)
    tour = list(range(n))
    np.random.shuffle(tour)
    cost = sum(dist[tour[i]][tour[(i+1) % n]] for i in range(n))
    best_tour, best_cost = tour[:], cost
    T = T0
    for k in range(n_iter):
        i, j = sorted(np.random.randint(0, n, size=2))  # 2-opt: pick segment
        if i == j: continue
        new_tour = tour[:i] + tour[i:j+1][::-1] + tour[j+1:]  # reverse it
        new_cost = sum(dist[new_tour[a]][new_tour[(a+1)%n]] for a in range(n))
        delta = new_cost - cost
        if delta < 0 or np.random.random() < np.exp(-delta / T):   # Metropolis
            tour, cost = new_tour, new_cost
            if cost < best_cost:
                best_tour, best_cost = tour[:], cost
        T *= alpha
    return best_tour, best_cost
```

20 lines of Python. No solver, no callbacks, no subtour constraints. Just a loop.

SA vs. B&B for TSP: The Tradeoff

	B&B + Lazy Cuts (Lec. 9)	**Simulated Annealing**
Solution quality	Provably optimal	Good (within 2–5%)
Scalability	$n \lesssim 200$	$n \sim 10{,}000+$
Running time	Exponential worst-case	User-controlled
Implementation	ILP + callbacks	20-line loop
Needs Gurobi?	Yes	No

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The deal: SA gives up the *proof* of optimality in exchange for being able to handle problems that B&B cannot touch. For TSP, SA tours are typically within 2–5% of optimal, which is good enough for many applications.

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The deal: SA gives up the *proof* of optimality in exchange for being able to handle problems that B&B cannot touch. For TSP, SA tours are typically within 2–5% of optimal, which is good enough for many applications.

Rule of thumb: if *n* is small enough for B&B and you need a certificate, use B&B. If you need a good solution on a large instance in bounded time, use SA.

From One Solution to a Population

SA maintains a **single** solution and perturbs it. This works well, but it explores one path at a time.

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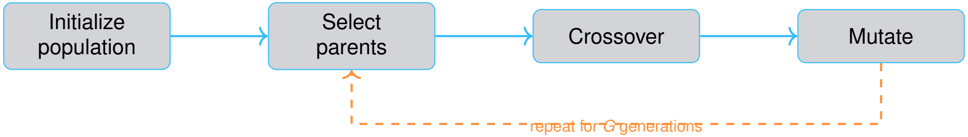
Key insight: if two decent solutions have different “good parts,” combining them might produce something better than either parent.

GA: The Pipeline



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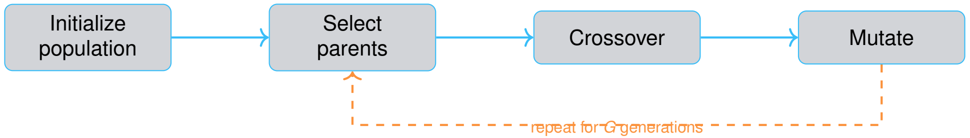

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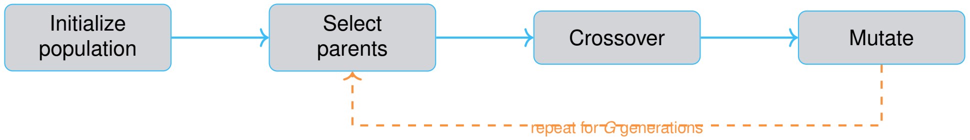

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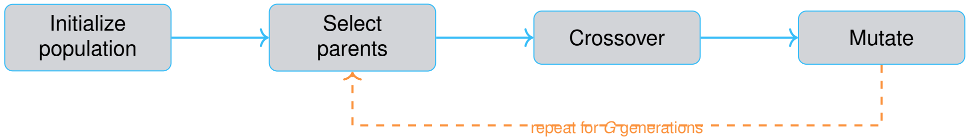

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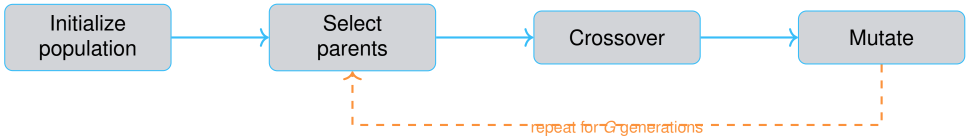

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4. **Elitism:** always keep the best few individuals from the previous generation.

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But: for **combinatorial** problems, we can't just average two permutations. The average of $(1,2,3,4,5)$ and $(5,4,3,2,1)$ is not a valid tour. We need something smarter.

The Problem with Naive Crossover on Permutations

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3 and 1 appear twice! Cities 2,5 missing!

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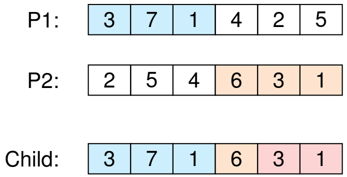

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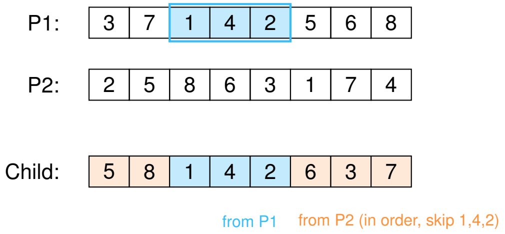

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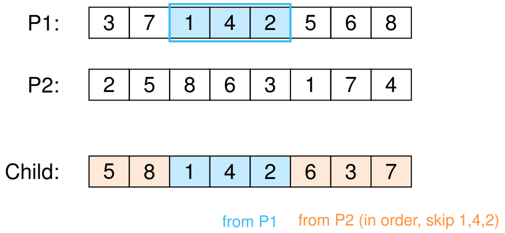

The child is a valid permutation. Cities $\{1, 4, 2\}$ come from P1; the rest are filled from P2's ordering.

Order Crossover: Code

```python
def order_crossover(p1, p2):
    n = len(p1)
    i, j = sorted(np.random.choice(n, 2, replace=False))
    child = [None] * n
    child[i:j+1] = p1[i:j+1]                        # copy segment from P1
    used = set(child[i:j+1])
    fill = [c for c in p2 if c not in used]          # P2 cities, in order, skip used
    pos = 0
    for k in range(n):
        if child[k] is None:
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Observation: the child inherits *local structure* (a contiguous segment) from P1, and *global ordering* from P2. If both parents have good sub-tours, the child has a chance of combining them.

GA for TSP: Putting It All Together

```python
def tsp_ga(dist, pop_size=100, n_gen=1000, mut_rate=0.02):
    n = len(dist)
    pop = [list(np.random.permutation(n)) for _ in range(pop_size)]
    cost = lambda t: sum(dist[t[i]][t[(i+1) % n]] for i in range(n))
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    for gen in range(n_gen):
        pop.sort(key=cost)
        new_pop = pop[:10]                          # elitism: keep top 10
        while len(new_pop) < pop_size:
            # tournament selection: pick 2 from top 20
            p1, p2 = [pop[np.random.randint(20)] for _ in range(2)]
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            child = order_crossover(p1, p2)        # crossover

            if np.random.random() < mut_rate:      # mutation: swap two cities
                a, b = np.random.choice(n, 2, replace=False)
                child[a], child[b] = child[b], child[a]
            new_pop.append(child)
        pop = new_pop
    pop.sort(key=cost)
    return pop[0], cost(pop[0])
```

SA vs. GA: When to Use Which?

	Simulated Annealing	**Genetic Algorithm**
# of solutions	One	Population
Exploration source	Temperature	Crossover + mutation
Parameters to tune	T_0, α, iterations	Pop size, rates, selection
Parallelism	Limited	Natural (eval pop. in parallel)

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- SA is often the **first thing to try**. Simpler, fewer parameters, surprisingly effective.
- GA shines when good sub-solutions can be meaningfully **recombined**.
- Both are dramatically outperformed by **problem-specific heuristics** when available (e.g., Lin–Kernighan for TSP). Metaheuristics are general-purpose. That's their strength and their weakness.

Why Hybrid?

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Two natural hybrids:

1. **SA $\rightarrow$ GD:** metaheuristic finds the right basin, GD refines to high precision.
2. **SA $\rightarrow$ Gurobi:** metaheuristic provides a strong incumbent, Gurobi proves optimality faster.

Hybrid 1: SA + GD on Rastrigin

Phase 1: SA for global exploration (find the right basin).
Phase 2: gradient descent for local refinement (converge precisely).

```python
# Phase 1: SA (rough search)
x = np.random.uniform(-5, 5, size=2)
T = 10.0
for k in range(200_000):
    x_new = x + np.random.randn(2) * 0.5
    delta = rastrigin(x_new) - rastrigin(x)
    if delta < 0 or np.random.random() < np.exp(-delta / T):
        x = x_new
    T *= 0.99997
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# Phase 2: GD refinement (starting from SA's answer)    <-- only new thing
x_t = torch.tensor(x, dtype=torch.float64, requires_grad=True)
opt = torch.optim.Adam([x_t], lr=0.01)
for _ in range(1000):
    loss = 10*2 + (x_t**2 - 10*torch.cos(2*torch.pi*x_t)).sum()
    opt.zero_grad(); loss.backward(); opt.step()
print(x_t.detach().numpy())   # [~0.0, ~0.0]
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SA gets us to the right neighborhood. GD polishes the answer.

Hybrid 2: SA Warm-Starts for Gurobi

Recall from Lecture 5: B&B prunes branches using the **incumbent** (best integer solution found so far). A better incumbent $\Rightarrow$ more pruning $\Rightarrow$ smaller search tree.

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"Hey Gurobi, I have this TSP model with lazy cuts, just like Lecture 9. But before you start, here's a tour I found with SA. It costs 1,847. Start from here. You don't have to search the whole tree, just prove you can't do better than 1,847 (or find something that does)."

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Result: Gurobi still proves optimality, but the search tree can be dramatically smaller because it starts with a strong bound.

Warm-Starting Gurobi: Code

```python
# Phase 1: SA finds a good tour (seconds)
sa_tour, sa_cost = tsp_sa(dist, n_iter=500_000)

# Phase 2: Set up ILP (same as Lecture 9)
m = gp.Model("TSP")
x = {}
for i in range(n):
    for j in range(n):
        if i != j:
            x[i,j] = m.addVar(vtype='B', name=f"x_{i}_{j}")
# ... degree constraints, lazy callbacks, etc. (same as Lecture 9) ...
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# New!! Feed SA solution as initial incumbent
for k in range(n):
    i = sa_tour[k]
    j = sa_tour[(k + 1) % n]
    x[i, j].Start = 1.0                  # hint: this arc is in the tour

m.optimize()    # Gurobi starts with sa_cost as initial UB --> prunes faster
```

Warm-Starting Gurobi: Code

```
# Phase 1: SA finds a good tour (seconds)
sa_tour, sa_cost = tsp_sa(dist, n_iter=500_000)

# Phase 2: Set up ILP (same as Lecture 9)
m = gp.Model("TSP")
x = {}
for i in range(n):
    for j in range(n):
        if i != j:
            x[i,j] = m.addVar(vtype='B', name=f"x_{i}_{j}")
# ... degree constraints, lazy callbacks, etc. (same as Lecture 9) ...

# New!! Feed SA solution as initial incumbent
for k in range(n):
    i = sa_tour[k]
    j = sa_tour[(k + 1) % n]
    x[i, j].Start = 1.0                  # hint: this arc is in the tour

m.optimize()    # Gurobi starts with sa_cost as initial UB --> prunes faster
```

The `.Start` attribute is the hint mechanism. Gurobi verifies feasibility and uses the solution as its initial incumbent if valid.