Discrete optimization

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Outline

- Definition of discrete optimization
- Combinatorial optimization
- Mixed-integer linear programming
- SAT solvers (Boolean satisfiability problem)
- Evolutionary algorithms (again)

Definition of discrete optimization

- Some (or all) variables values are in $\mathbb{Z}$ or $\mathbb{N}$
  - It is commonly assumed that variable values can be sorted
  - If we can enumerate all candidates, **combinatorial optimization**

- Example: mixed integer sphere

$$f(x_1, x_2) = x_1^2 + x_2^2 \text{ where } x_1 \in \mathbb{R}, x_2 \in \mathbb{Z}$$

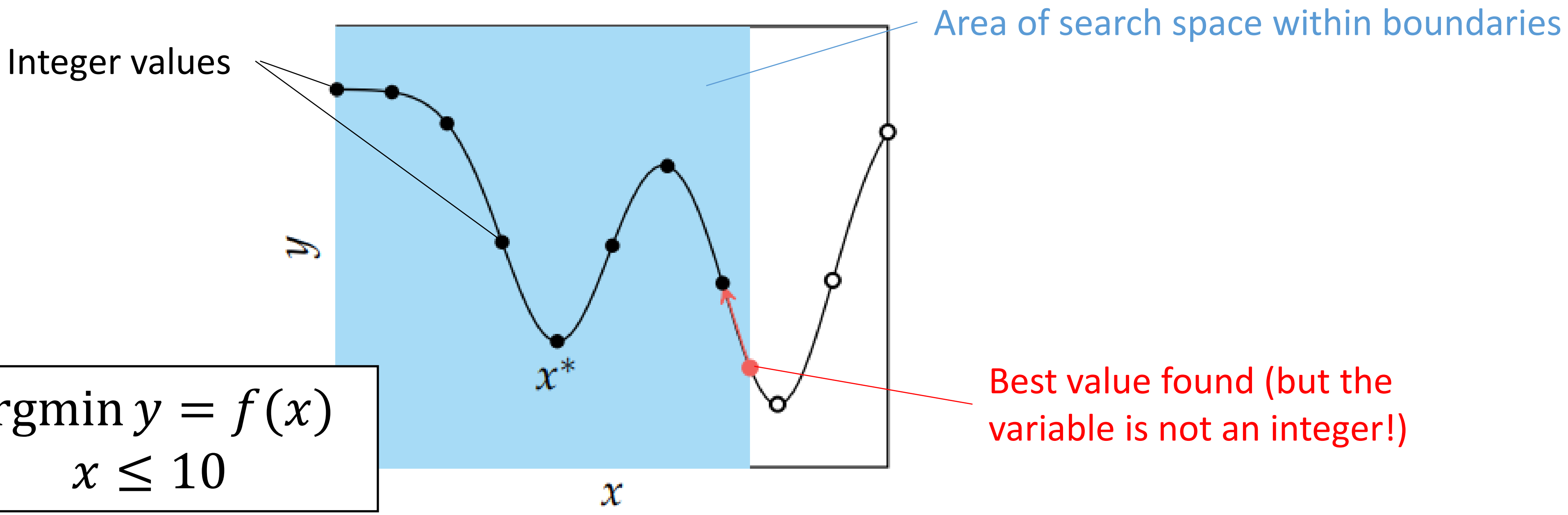
Definition of discrete optimization

- Variable values could also be **categorical**
  - E.g. x={red, green, blue}; there is no default way of sorting
  - Some algorithms can manage them natively
  - Others encode them as **bitstrings** with constraints
  - In ML sometimes called “one-hot encoding”

- Example: $x \rightarrow x_r, x_g, x_b \in \{0,1\}; x_r + x_g + x_b = 1$

Discrete optimization

- Trivial (and *ineffective*) solution
  - "Relax" the problem into a continuous one
  - Round up variable values of best solution to the closest integer



$$\begin{gathered}\operatorname{argmin} y = f(x) \\ x \leq 10\end{gathered}$$

Branch and bound

- If you can enumerate all possible solutions of a problem
- Exhaustive approach: evaluate them all, find global optimum
- Branch & Bound guarantees finding the global optimum
  - Without exploring everything, creates a tree
  - Branch: divide search space into partitions with extra constraints
  - Bound: compute lower bound for a partition, linear programming
  - Pruning: decide what branches are not worthy of being explored

Branch and bound

$$\textbf{argmax } \boldsymbol{f}(\boldsymbol{x_1}, \boldsymbol{x_2}) = \mathbf{5}\boldsymbol{x_1} + \mathbf{6}\boldsymbol{x_2}$$
$$x_1 + x_2 \leq 5$$
$$4x_1 + 7x_2 \leq 28$$
$$x_1, x_2 \geq 0$$
$$x_1, x_2 \in \mathbb{N}$$

Branch and bound

$$f(x_1, x_2) = 27.67$$
$$x_1 = 2.33$$
$$x_2 = 2.67$$

$$\mathbf{argmax}\ \boldsymbol{f(x_1, x_2) = 5x_1 + 6x_2}$$
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$f(x_1, x_2) = 27$
$x_1 = 3$
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$x_2 \geq 3$

$f(x_1, x_2) = 26.75$
$\boldsymbol{x_1 = 1.75}$
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Branch and bound

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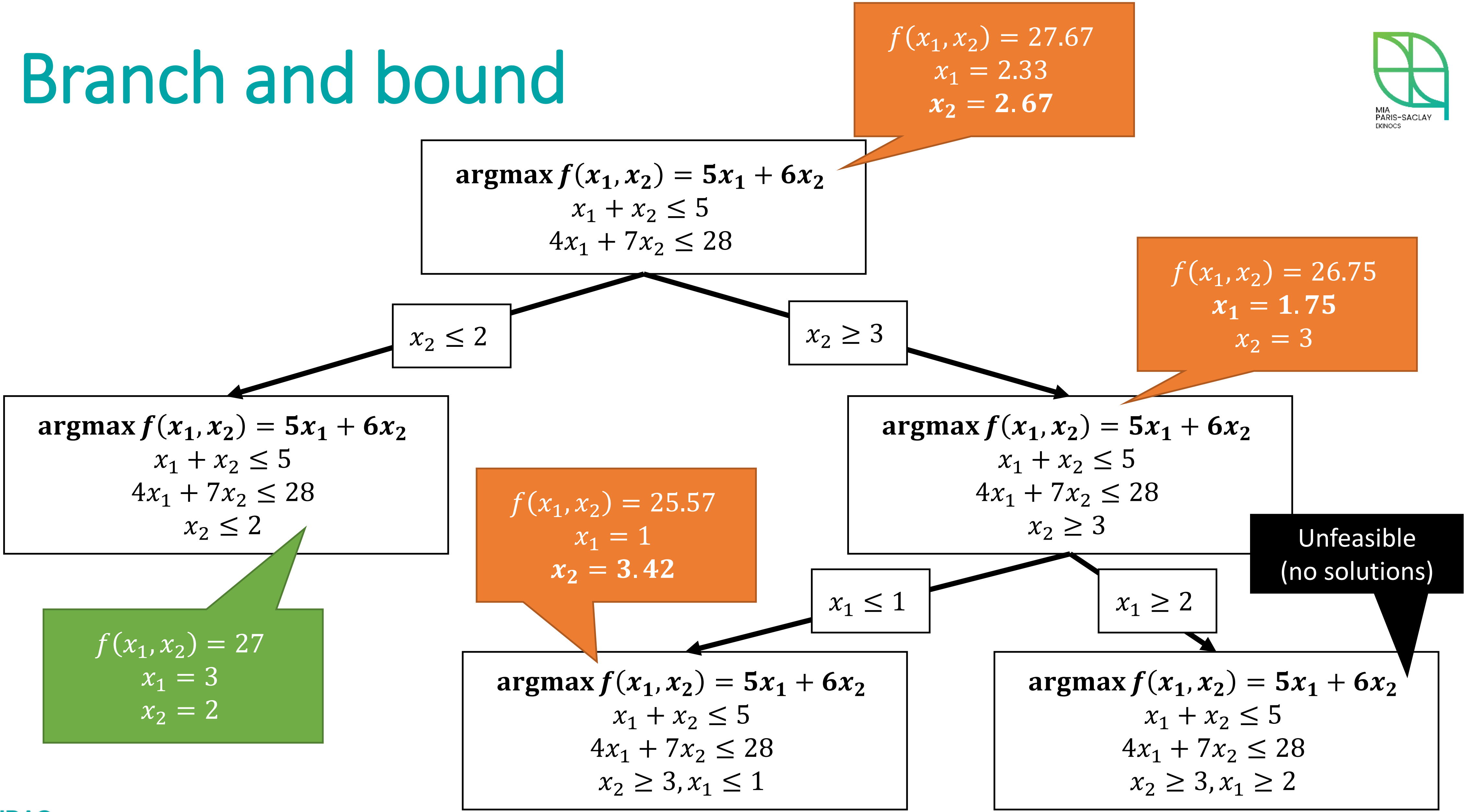
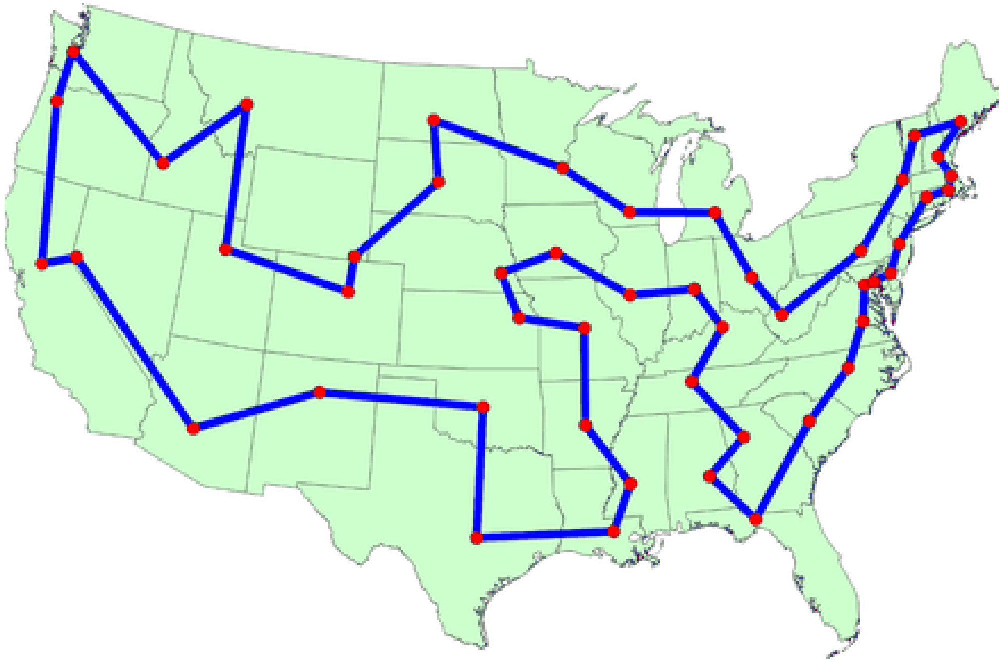
Branch and bound



Traveling salesman problem

- Salesman has to visit multiple cities once, in any order
- What is the optimal order, to minimize total time?



Traveling salesman problem

- Combinatorial: compute total number of possible paths

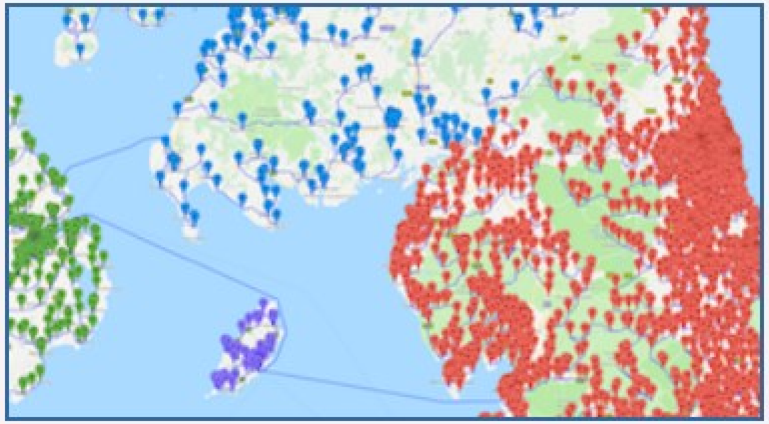
$$n_p = \frac{(n_c - 1)!}{2}$$

- With n_c being the number of cities
  - For 30 cities, 4.42 x 10^{30} possible paths
  - For 100 cities, 4.67 x 10^{155}
  - For 1,000 cities, 2.01 x 10^{249}
- Estimated number of atoms in the universe: 10^{78} - 10^{82}

Traveling salesman problem

- The best algorithm is (arguably) *heuristic*
  - Mix of linear programming, evolutionary algorithms, …
  - CONCORDE: https://www.math.uwaterloo.ca/tsp/index.html

Winning $100,000 in the Amazon Last Mile Routing Research Challenge.

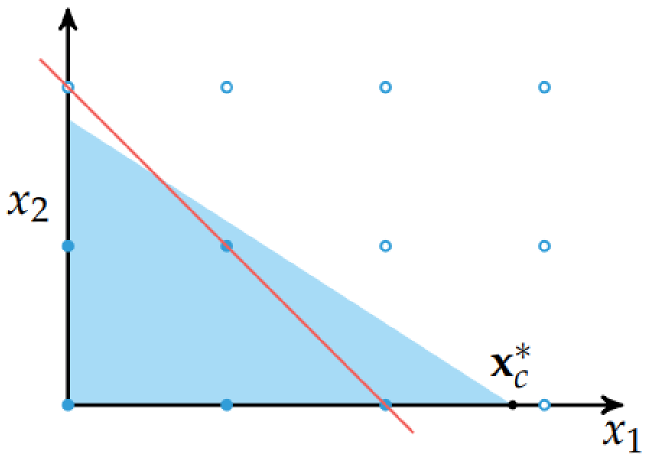


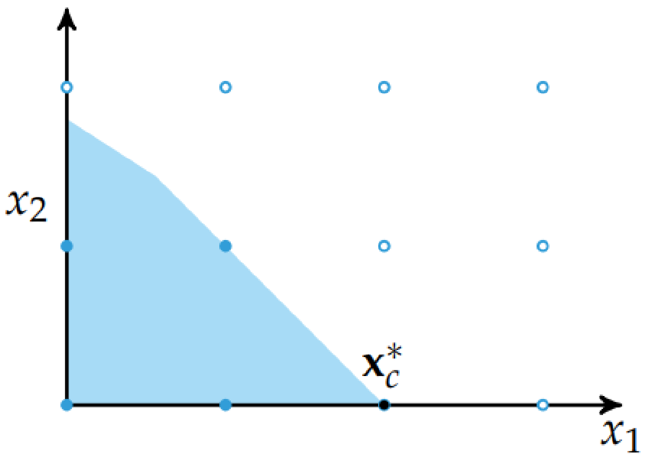
Optimal crawl to 49,687 pubs in the UK.

Visit 49,603 historic sites in the US.

Mixed-integer linear programming

- MILP: Class of problems with different solvers
- Example: Branch-and-cut
  - Similar to Branch and Bound + cutting planes (multiple variables)
  - Different strategies to find best possible cutting planes





Boolean satisfiability (SAT solvers)

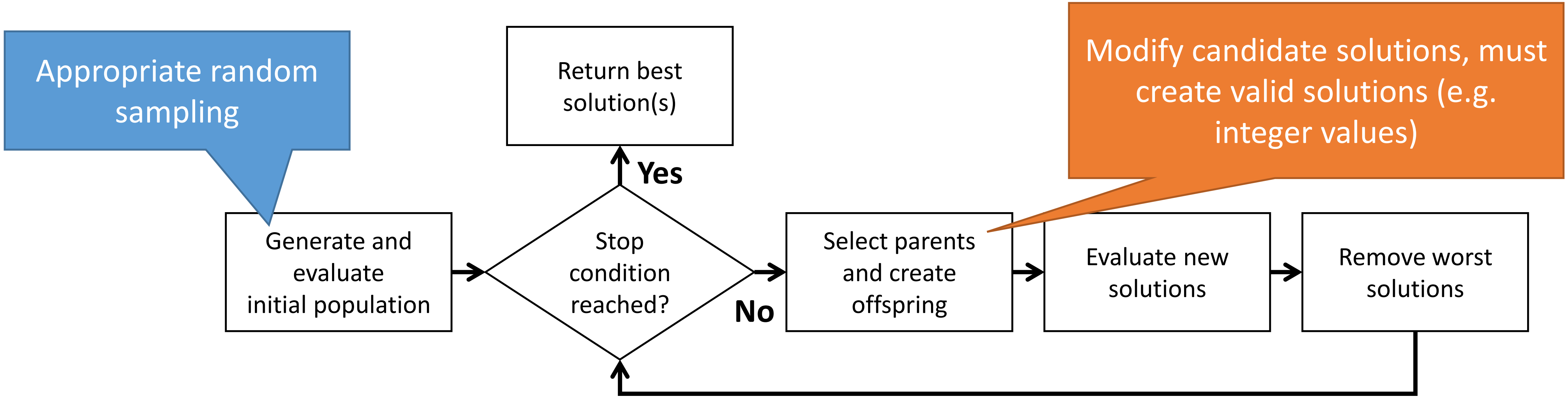
- Boolean expression (binary variables)
- Existence of a candidate solution that outputs *true*?

$$f(\mathbf{x}) = x_1 \wedge (x_2 \vee \neg x_3) \wedge (\neg x_1 \vee \neg x_2)$$

- Complex problem
- Specialized techniques called SAT solvers

Evolutionary algorithms (again)

- Internal representation of a candidate solution mixed integer
  - Requires problem-specific variators (int for int parameters, …)
  - But in general, it's relatively straightforward
  - No guarantee to find the global optimum



Questions?

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