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Heuristic Search

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Winter 2009

Heuristic Search

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Heuristic Search Intro

Heuristic Search vs Exhaustive Search

Exhaustive Search

- Backtracking (backtracking with bounding):
 - Find all feasible solutions.
 - Find one optimal solution.
 - Find all optimal solutions.
- Branch-and-Bound:
 - Find one optimal solution.

Heuristic Search

Types of problem it can be applied to:

- Find 1 optimal solution (when optimum value is known)
- Find a "close to" optimal solution (the best solution we manage).

Heuristics methods we will study:

• Hill-climbing, Simulated annealing, Tabu search, Genetic algorithms.

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Heuristic Search Intro

Characteristics of heuristic search

- The state space is not fully explored.
- Randomization is often employed.
- There is a concept of neighbourhood search.
- **Heuristics** are applied to explore the solutions. The word "heuristics" means "serving or helping to find or discover" or "proceeding by trial and error".

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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A general framework for heuristic search

Generic Optimization Problem (maximization):

Exercise: pick your favorite combinatorial optimization problem and write it in this framework.

Heuristic Search Intro	Design Strategies for Heuristic Algorithms 00 000000 000000	Heuristic Searches Applied to Various Problems 0000000 000000 0000000000
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A general framework for heuristic search (cont'd)

Designing a heuristic search:

- Define a **neighbourhood function** $N : \mathcal{X} \to 2^{\mathcal{X}}$. E.g. $N(X) = \{X_1, X_2, X_3, X_4, X_5\}.$
- Obesign a neighbourhood search: Algorithm that finds a feasible solution on the neighbourhood of a feasible solution X.

There are two types of neghbourhood searches:

- Exhaustive (chooses best profit among neighbour points)
- Randomized (picks a random point among the neighbour points)

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Defining a neighbourhood function

 $N: \mathcal{X} \to 2^{\mathcal{X}}.$

So, N(X) is a subset of \mathcal{X} .

• N(X) should contain elements that are similar or "close to" X.

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Defining a neighbourhood function

 $N: \mathcal{X} \to 2^{\mathcal{X}}.$

- N(X) should contain elements that are similar or "close to" X.
- N(X) may contain infeasible elements of \mathcal{X} .

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Defining a neighbourhood function

 $N: \mathcal{X} \to 2^{\mathcal{X}}.$

- N(X) should contain elements that are similar or "close to" X.
- N(X) may contain infeasible elements of \mathcal{X} .
- In order to be useful, we would like to be able to get to X_{opt} from X_0 via a number of applications of $N(\cdot)$.

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Defining a neighbourhood function

 $N: \mathcal{X} \to 2^{\mathcal{X}}.$

- N(X) should contain elements that are similar or "close to" X.
- N(X) may contain infeasible elements of \mathcal{X} .
- In order to be useful, we would like to be able to get to X_{opt} from X₀ via a number of applications of N(·).
- I.E. the graph G with $V(G) = \mathcal{X}$ and $E(G) = \{\{X, Y\} : Y \in N(X)\}$ should ideally be connected, or at least have one optimal solution in each of its connected components.

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Defining a neighbourhood function

 $N: \mathcal{X} \to 2^{\mathcal{X}}.$

- N(X) should contain elements that are similar or "close to" X.
- N(X) may contain infeasible elements of \mathcal{X} .
- In order to be useful, we would like to be able to get to X_{opt} from X_0 via a number of applications of $N(\cdot)$.
- I.E. the graph G with $V(G) = \mathcal{X}$ and $E(G) = \{\{X, Y\} : Y \in N(X)\}$ should ideally be connected, or at least have one optimal solution in each of its connected components.
- \bullet Computing N(X) should be fast, and in particular |N(X)| shouldn't be too large.

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Examples of neighbourhood functions

First, define dist(X, Y) for $X, Y \in \mathcal{X}$. Let d_0 be a constant positive integer. We can define a neighbourhood function as follows:

 $N_{d_0}(X) = \{ Y \in \mathcal{X} : dist(X, Y) \le d_0 \}.$

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Examples of neighbourhood functions based on distances

• $\mathcal{X} = \{0, 1\}^n$, set of all binary *n*-tuples. Here *dist* is the Hamming distance. $N_1([010]) = \{[000], [110], [011], [010]\}.$

$$|N_{d_0}(X)| = \sum_{i=0}^{d_0} \binom{n}{i}.$$

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Examples of neighbourhood functions based on distances

• $\mathcal{X} = \{0, 1\}^n$, set of all binary *n*-tuples. Here *dist* is the Hamming distance. $N_1([010]) = \{[000], [110], [011], [010]\}.$

$$|N_{d_0}(X)| = \sum_{i=0}^{d_0} \binom{n}{i}.$$

• $\mathcal{X} = \text{set of all permutations of } \{1, 2, \dots, n\}.$ Let $\alpha = [\alpha_1, \dots, \alpha_n]$ and $\beta = [\beta_1, \dots, \beta_n]$ be two permutations. Define distance as follows: $dist(\alpha, \beta) = |\{i : \alpha_i \neq \beta_i\}|.$ Note that $N_1(X) = \{X\}$ is not very useful; we need $d_0 > 1.$ $N_2([1, 2, 3, 4]) = \{[1, 2, 3, 4], [2, 1, 3, 4], [3, 2, 1, 4], [4, 2, 3, 1], [1, 3, 2, 4], [1, 4, 3, 2], [1, 2, 4, 3]\}$ $|N_2(X)| = 1 + \binom{n}{2}.$

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Designing a neighbourhood search algorithm

Designing a neighbourhood search algorithm Input: X

Output: $Y \in N(X) \setminus \{X\}$ such that Y is feasible, or "fail". Possible Neighbourhood Search Strategies:

- Find a feasible $Y \in N(X) \setminus \{X\}$ such that P(Y) is maximized. Return "fail" if there is no feasible solution in $N(X) \setminus \{X\}$.
- ② Find a feasible Y ∈ N(X) \ {X} such that P(Y) is maximized. if P(Y) > P(X) then return Y; else return "fail". (steepest ascent method)
- Find any feasible Y ∈ N(X) \ {X}.
 Return "fail" if there is no feasible solution in N(X) \ {X}.
- Find any feasible $Y \in N(X) \setminus \{X\}$.
 - if P(Y) > P(X) then return Y; else return "fail".

Strategies 1 and 2 may be exhaustive.

Strateges 3 and 4 are usually randomized.

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Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Designing a neighbourhood search algorithm

A generic heuristic search algorithm

Given N, a neighbourhood function, the heuristic algorithm h_N either:

- Perform one neighbourhood search (using one of the strategies)
- Perform a sequence of *j* neighbourhood searches, where each one takes us from X_i to X_{i+1} : $[X = X_0, X_1, \dots, X_j = Y]$.

Algorithm GENERICHEURISTICSEARCH(c_{max}) Select a feasible solution $X \in \mathcal{X}$; $X_{best} \leftarrow X$; (stores best so far); $c \leftarrow 0$; while $(c \leq c_{max})$ do $Y \leftarrow h_N(X)$; if $(Y \neq$ "fail") then $X \leftarrow Y$; if $(P(X) > P(X_{best}))$ then $X_{best} \leftarrow X$; [else $c \leftarrow c_{max} + 1$; (add this if h_N is not randomized)] $c \leftarrow c + 1$; return X_{best} ;

Heuristic Search

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Hill-Climbing		

• Idea: Go up the hill continuously, stop when stuck.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Hill-Climbing		

- Idea: Go up the hill continuously, stop when stuck.
- Problem: it can get stuck in a local optimum.

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Hill-Climbing		

- Idea: Go up the hill continuously, stop when stuck.
- Problem: it can get stuck in a local optimum.
- Improvement: run the algorithm many times from different random starting points *X*.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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fill-Climbing		

- Idea: Go up the hill continuously, stop when stuck.
- Problem: it can get stuck in a local optimum.
- Improvement: run the algorithm many times from different random starting points X.
- For Hill-Climbing, $h_N(X)$ returns:

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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II-Climbing		

- Idea: Go up the hill continuously, stop when stuck.
- Problem: it can get stuck in a local optimum.
- Improvement: run the algorithm many times from different random starting points X.
- For Hill-Climbing, $h_N(X)$ returns:
 - $Y \in N(X)$ such that Y is feasible and P(Y) > P(X),

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I-Climbing		

- Idea: Go up the hill continuously, stop when stuck.
- Problem: it can get stuck in a local optimum.
- Improvement: run the algorithm many times from different random starting points X.
- For Hill-Climbing, $h_N(X)$ returns:
 - $Y \in N(X)$ such that Y is feasible and P(Y) > P(X),
 - or, otherwise, "fail".

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Hill-Climbing

Hill Climbing Algorithm

```
Algorithm GENERICHILLCLIMBING()

Select a feasible solution X \in \mathcal{X}.

X_{best} \leftarrow X; searching \leftarrow true;

while (searching) do

Y \leftarrow h_N(X);

if (Y \neq \text{``fail''}) then

X \leftarrow Y;

if (P(X) > P(X_{best})) then X_{best} \leftarrow X;

else searching \leftarrow false;

return X_{best};
```

rategies for Heuristic Algorithms

Hill-climbing can get trapped in a local optimum. Other search strategies (**simulated annealing,tabu search**) try to escape from local optima.

Heuristic Search

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Simulated Annealing		

• Analogy with a method of cooling metal: annealing.



	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Simulated Appealing	00000	

- Analogy with a method of cooling metal: annealing.
 - Temperature T decreases at each iteration, according to a cooling schedule (T₀, α):

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Cimulated Annealing		

- Analogy with a method of cooling metal: annealing.
 - Temperature T decreases at each iteration, according to a cooling schedule (T₀, α):
 - Initally $T \leftarrow T_0$;

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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- Analogy with a method of cooling metal: annealing.
 - Temperature T decreases at each iteration, according to a cooling schedule (T₀, α):
 - Initally $T \leftarrow T_0$;
 - later $T \leftarrow \alpha T$ for a fixed $0 < \alpha < 1$.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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- Analogy with a method of cooling metal: annealing.
 - Temperature T decreases at each iteration, according to a cooling schedule (T₀, α):
 - Initally $T \leftarrow T_0$;
 - later $T \leftarrow \alpha T$ for a fixed $0 < \alpha < 1$.
- Going uphill is always accepted.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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- Analogy with a method of cooling metal: annealing.
 - Temperature T decreases at each iteration, according to a cooling schedule (T₀, α):
 - Initally $T \leftarrow T_0$;
 - later $T \leftarrow \alpha T$ for a fixed $0 < \alpha < 1$.
- Going uphill is always accepted.
- Going downhill is sometimes accepted with a probability based on how much downhill we go and on the current temperature.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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- Analogy with a method of cooling metal: annealing.
 - Temperature T decreases at each iteration, according to a cooling schedule (T₀, α):
 - Initally $T \leftarrow T_0$;
 - later $T \leftarrow \alpha T$ for a fixed $0 < \alpha < 1$.
- Going uphill is always accepted.
- Going downhill is sometimes accepted with a probability based on how much downhill we go and on the current temperature.
 - Given $Y = h_N(X)$ with $P(Y) \le P(X)$,

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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- Analogy with a method of cooling metal: annealing.
 - Temperature T decreases at each iteration, according to a cooling schedule (T₀, α):
 - Initally $T \leftarrow T_0$;
 - later $T \leftarrow \alpha T$ for a fixed $0 < \alpha < 1$.
- Going uphill is always accepted.
- Going downhill is sometimes accepted with a probability based on how much downhill we go and on the current temperature.
 - Given $Y = h_N(X)$ with $P(Y) \le P(X)$,
 - accept Y with probability

$$e^{(P(Y)-P(X))/T} = \frac{1}{e^{(P(X)-P(Y))/T}}$$

(We get pickier as we progress, since T decreases)

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Simulated Annealing Algorithm

Algorithm GENERICSIMULATEDANNEALING (c_{max}, T_0, α) $c \leftarrow 0$: $T \leftarrow T_0$: Select a feasible solution $X \in \mathcal{X}$; $X_{best} \leftarrow X$; while $(c < c_{max})$ do $Y \leftarrow h_N(X)$; // this is usually a randomized choice if $(Y \neq \text{``fail''})$ then if (P(Y) > P(X)) then $X \leftarrow Y$: if $(P(X) > P(X_{best}))$ then $X_{best} \leftarrow X$; else $r \leftarrow random(0, 1)$; if $(r < e^{\frac{P(Y) - P(X)}{T}})$ then $X \leftarrow Y$: $c \leftarrow c + 1$: $T \leftarrow \alpha T$: return X_{hest} :

Heuristic Search

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

• Neighbourhood search:

Choose $Y \in N(X) \setminus \{X\}$ such that Y is feasible and P(Y) is maximum among all such elements (exhaustive neighbourhood search).

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

• Neighbourhood search:

Choose $Y \in N(X) \setminus \{X\}$ such that Y is feasible and P(Y) is maximum among all such elements (exhaustive neighbourhood search).

It may happen that P(Y) < P(X) (we escape from a local optimum).

• What may be the risk?

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

• Neighbourhood search:

Choose $Y \in N(X) \setminus \{X\}$ such that Y is feasible and P(Y) is maximum among all such elements (exhaustive neighbourhood search).

- What may be the risk?
 - Cycling.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

• Neighbourhood search:

Choose $Y \in N(X) \setminus \{X\}$ such that Y is feasible and P(Y) is maximum among all such elements (exhaustive neighbourhood search).

- What may be the risk?
 - Cycling.
 - When going downhill from X to Y we may go back from X to Y.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

• Neighbourhood search:

Choose $Y \in N(X) \setminus \{X\}$ such that Y is feasible and P(Y) is maximum among all such elements (exhaustive neighbourhood search).

- What may be the risk?
 - Cycling.
 - When going downhill from X to Y we may go back from X to Y.
 - Cycling may also take several steps, such as $X \to Y \to Z \to X$.
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Tabu Search

• Neighbourhood search:

Choose $Y \in N(X) \setminus \{X\}$ such that Y is feasible and P(Y) is maximum among all such elements (exhaustive neighbourhood search).

It may happen that P(Y) < P(X) (we escape from a local optimum).

- What may be the risk?
 - Cycling.
 - ▶ When going downhill from X to Y we may go back from X to Y.
 - Cycling may also take several steps, such as $X \to Y \to Z \to X$.
- Tabu-search uses a strategy for avoiding cycling: a **tabu list**. After a move $X \to Y$, we forbit the application of CHANGE(Y, X) for L iterations (L is the lifetime of the tabu list).

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

Tabu List

• After a move $X \to Y$, we keep CHANGE(Y, X) t the Tabu List for L iterations.

Heuristic Search Intro 00 00000	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

Tabu List

- After a move $X \to Y$, we keep CHANGE(Y, X) t the Tabu List for L iterations.
- Example:

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

Tabu List

- After a move $X \to Y$, we keep CHANGE(Y, X) t the Tabu List for L iterations.
- Example:
 - $\begin{array}{l} \mathcal{X} = \{0,1\}^n, \text{ using } N_1(X) = \{Y \in \mathcal{X} : dist(X,Y) = 1\}. \\ X = [0100] \text{ and } Y = [0101], \text{ we have that } \mathrm{CHANGE}(Y,X) = 4 = \\ \mathrm{index \ of \ coordinate \ that \ was \ swapped.} \\ \mathrm{Suppose \ } L = 2. \\ \mathrm{sequence \ of \ points:} \ \left| \begin{array}{c} [0100] \\ 4 \end{array} \right| \begin{array}{c} [0101] \\ [1011] \\ 4 \end{array} \right| \begin{array}{c} [1001] \\ 1,2 \end{array} \right| \begin{array}{c} [1011] \\ 2,3 \end{array} \right|$
- So any sequence that cycles $X \to \ldots \to X$ has length at least 2L. Choosing L = 10 is typical.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

TABULIST is defined below to be a list where TABULIST[c] = δ , where δ is the designated forbidden (tabu) change at iteration c.

For tabu search, $h_N(X) = Y$, where

- $Y \in N(X)$, Y is feasible;
- CHANGE $(X, Y) \notin \{ \text{ TABULIST}[d] : c L \le d \le c 1 \};$
- P(Y) is maximum among all such feasible elements.

In absolute no circumstance implement TABULIST as an array indexed by the number of iterations! Instead, implement TABULIST as a queue of length L. Note that the algorithm may mislead you to think you are using such an array, given the notation defined above; careful!

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

Tabu Search Algorithm: textbook version/typo correction

Algorithm GENERICTABUSEARCH (c_{max}, L) $c \leftarrow 1$: Select a feasible solution $X \in \mathcal{X}$. $X_{hest} \leftarrow X;$ while $(c < c_{max})$ do $N \leftarrow N(X) \setminus \{F : \text{CHANGE}(X, F) \in \text{TABULIST}[d], c - L \le d \le c - 1\};$ for each $(Y \in N)$ do if (Y is infeasible) then $N \leftarrow N \setminus \{Y\}$; if $(N = \emptyset)$ then return X_{best} ; Find $Y \in N$ such that P(Y) is maximum; /* computes $Y = h_N(X) * /$ TABULIST $[c] \leftarrow CHANGE(Y, X);$ $X \leftarrow Y$: if $(P(X) > P(X_{best}))$ then $X_{best} \leftarrow X$; $c \leftarrow c + 1$: return X_{best} ;

Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Tabu Search		

Tabu List Implementation

In absolute no circumstance implement ${\rm TABULIST}$ as an array indexed by the number of iterations!

In the real implementation, TABULIST can be a queue of length L!!! So, the operation

TABULIST
$$[c] \leftarrow CHANGE(Y, X);$$

must be implemented as:

TABULIST.insert(CHANGE(Y, X)); (only keeps last L elements) and the line: $N \leftarrow N(X) \setminus \{F :$ CHANGE $(X, F) \in \text{TABULIST}[d], c - L \le d \le c - 1\}$ should be understood as:

 $N \leftarrow N(X) \setminus \{F : CHANGE(X, F) \text{ is in TABULIST}\};$

Heuristic Search Intro 00 00000 00	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems 000000000 0000000 000000000
Tabu Search		

Tabu Search Algorithm: with FIFO queue for TABULIST

```
Algorithm GENERICTABUSEARCH(c_{max}, L)
  c \leftarrow 1:
  Select a feasible solution X \in \mathcal{X}.
  X_{hest} \leftarrow X;
  while (c < c_{max}) do
      N \leftarrow N(X) \setminus \{F : \text{CHANGE}(X, F) \text{ is in TABULIST}\}
      for each (Y \in N) do if (Y is infeasible) then N \leftarrow N \setminus \{Y\};
      if (N = \emptyset) then return X_{hest};
      Find Y \in N such that P(Y) is maximum; /* computes Y = h_N(X) */
      TABULIST.insert(CHANGE(Y, X), L); /* only keeps last L entries */
      X \leftarrow Y:
      if (P(X) > P(X_{best})) then X_{best} \leftarrow X;
      c \leftarrow c + 1:
  return X_{best}:
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	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Genetic Algorithms		

Genetic Algorithms

Fix a number POPSIZE (population size). One iteration works as follows:



Iterate as many generations as you like.

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Mating Strategies (Recombination)

Producing children from parents.

Method 1: Crossover.

Let j be a crossover point.



	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Genetic Algorithms		

Mating Strategies (Recombination), cont'd

Method 2: Partially matched crossover (for permutations)

Two crossover points: $1 \le j < k \le n$		
Example: $j = 3$ and $k = 6$		
$\alpha = [3, 1, \underline{4, 7, 6, 5}, 2, 8] \qquad \beta = [8, 6, \underline{4, 3, 7, 1}, 2, 5]$		
swap	α	β
$4 \leftrightarrow 4$	$\left[3,1,4,7,6,5,2,8\right]$	[8, 6, 4, 3, 7, 1, 2, 5]
$7\leftrightarrow 3$	$\left[7,1,4,3,6,5,2,8\right]$	[8, 6, 4, 7, 3, 1, 2, 5]
$6 \leftrightarrow 7$	$\left[6,1,4,3,7,5,2,8\right]$	[8, 7, 4, 6, 3, 1, 2, 5]
$5\leftrightarrow 1$	[6, 5, 4, 3, 7, 1, 2, 8]	[8, 7, 4, 6, 3, 5, 2, 1]

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	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Genetic Algorithms		

Mating Schemes

Kids may be infeasible: incorporate constraints as penalties.

Various methods are possible for mating schemes:

- Random monogamy with 2 kids per couple: randomly partition population into pairs, with two kids produced by each pair.
- One of the second se

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Constic Algorithms		

Algorithm GENERICGENETICALGORITHM ($PopSize, c_{max}$) Select an initial population \mathcal{P} with PopSize feasible solutions; for each $X \in \mathcal{P}$ do $X \leftarrow h_N(X)$; [mutation] $X_{best} \leftarrow$ element in \mathcal{P} with maximum profit; $c \leftarrow 1$; while $(c < c_{max})$ do $\mathcal{Q} \leftarrow \mathcal{P}$; Construct a pairing of the elements in \mathcal{P} ; for each pair (W, X) in the pairing do $(Y,Z) \leftarrow rec(W,X);$ [recombination/mating] $Y \leftarrow h_N(Y); Z \leftarrow h_N(Z);$ [mutations] $\mathcal{Q} \leftarrow \mathcal{Q} \cup \{Y, Z\};$ Set \mathcal{P} to be the best *PopSize* members of \mathcal{Q} ; Let Y be the element in \mathcal{P} with maximum profit; if $(P(Y) > P(X_{best}))$ then $X_{best} \leftarrow Y$; $c \leftarrow c + 1$: return X_{hest} :

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Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Hill-climbing Algorithms

Steepest Ascent for Uniform Graph Partition

PROBLEM: UNIFORM GRAPH PARTITION INSTANCE: A COMPLETE GRAPH ON 2n VERTICES, $cost: E \to Z^+ \cup \{0\}$ (COST FUNCTION) FIND: THE MINIMUM VALUE OF $C([X_0, X_1]) = \sum_{u \in X_0, v \in X_1} cost(u, v)$ SUBJECT TO $V = X_0 \cup X_1, |X_0| = |X_1| = n.$

Example: n = 4; cost(1, 2) = 1, cost(1, 3) = 2, cost(1, 4) = 5, cost(2, 3) = 0, cost(2, 4) = 5, cost(3, 4) = 1.

Only 3 feasible solutions (except for exchanging X_0 and X_1):

$$\begin{aligned} X_0 &= \{1, 2\}, \quad X_1 &= \{3, 4\}, \qquad C([X_0, X_1]) = 12 \\ X_0 &= \{1, 3\}, \quad X_1 &= \{2, 4\}, \qquad C([X_0, X_1]) = 7 \quad (optimal) \\ X_0 &= \{1, 4\}, \quad X_1 &= \{2, 3\}, \qquad C([X_0, X_1]) = 9 \end{aligned}$$

Heuristic		

Design Strategies for Heuristic Algorithms 00 00000 000000 Heuristic Searches Applied to Various Problems

Hill-climbing Algorithms

Uniform Graph Partition: Steepest Ascend Algorithm

Neighbourhood function: exchange $x \in X_0$ and $y \in X_1$.

$$\begin{array}{l} \text{Algorithm UGP}(C_{max}) \\ X = [X_0, X_1] \leftarrow \text{SelectRandomPartition} \\ c \leftarrow 1 \\ \text{while } (c \leq C_{max}) \text{ do} \\ [Y_0, Y_1] \leftarrow \text{Ascend}(X) \\ \text{ if not fail then} \\ \{X_0 \leftarrow Y_0; \ X_1 \leftarrow Y_1; \} \\ \text{ else return} \\ c \leftarrow c + 1 \end{array}$$

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	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Ascend Algorithm

```
Algorithm Ascend([X_0, X_1])
      q \leftarrow 0
      for each i \in X_0 do
            for each j \in X_1 do
                   t \leftarrow G_{[X_0, X_1]}(i, j) (gain obtained in exchange)
                   if (t > q) then \{x \leftarrow i; y \leftarrow j; q \leftarrow t\}
      if (q > 0) then
          Y_0 \leftarrow (X_0 \cup \{y\}) \setminus \{x\}
          Y_0 \leftarrow (X_1 \cup \{x\}) \setminus \{y\}
           fail \leftarrow false
           return [Y_0, Y_1]
      else {fail \leftarrow true; return [X_0, X_1]}
```

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Design Strategies for Heuristic Algorithms 00 000000 000000 Heuristic Searches Applied to Various Problems

Hill-climbing Algorithms

SelectRandomPartition

Two possible algorithms:

- Picking X_0 as a random *n*-subset *r* of a 2n-set: Get a random integer $r \in [0, \binom{2n}{n} - 1]$ and apply kSubsetLexUnrank(r, n, 2n).
- Randomly shufling elements in [0, 2n 1]: Create array A[0, 2n - 1] with randomly chosen numbers as elements. Create array B[0, 2n - 1] initially with B[i] = i. Sort A, doing same swaps on B. Take X₀ as the first half of B, and X₁ as the second half.

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Design Strategies for Heuristic Algorithms DO DO DODOOO DOOOO Heuristic Searches Applied to Various Problems

Hill-climbing Algorithms

Hill-climbing for Steiner triple systems Textbook, Section 5.4.

Definition

A Steiner triple system of order v, denoted STS(v), is a pair (V, \mathcal{B}) where: $V = \{1, 2, \ldots v\}$ is a set of points, $\mathcal{B} = \{B_1, B_2, \ldots, B_b\}$ is a set of 3-sets, called blocks, such that any pair of points in V is in a unique block $B_i \in \mathcal{B}$.

Example: STS(9):

$$\begin{split} V &= & \{1,2,3,4,5,6,7,8,9\} \\ \mathcal{B} &= & \{ & \{1,2,3\},\{1,4,7\},\{1,5,9\},\{1,6,8\},\{4,5,6\},\{2,5,8\}, \\ & \{2,6,7\},\{2,4,9\},\{7,8,9\},\{3,6,9\},\{3,4,8\},\{3,5,7\} \} \end{split}$$

Heuristic	

Design Strategies for Heuristic Algorithms 00 000000 00000 Heuristic Searches Applied to Various Problems

Hill-climbing Algorithms

Replication number and number of blocks

Lemma

Let (V, \mathcal{B}) be an STS(v). Then, every point in V occurs in exactly $r = \frac{v-1}{2}$ blocks and $|\mathcal{B}| = \frac{v(v-1)}{6}$.

Proof:

- Any point x must appear in some block with each of all other (v-1) points. Point x occurs with 2 other points in each of the r_x blocks it appears. Therefore, $r_x = \frac{v-1}{2}$.
- **2** We count *T*, the number of points with their replications appearing on \mathcal{B} , in two ways: $T = 3 \times b$ and $T = v \times r$. Thus, $3 \times b = v \times r$, which implies $b = \frac{v(v-1)}{6}$.

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Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Hill-climbing Algorithms

Necessary and sufficient conditions for existence of STS(v)

Since $r = \frac{v-1}{2}$ (point replication number) and $b = \frac{v(v-1)}{6}$ (number of blocks) must be integer numbers, we need $v \equiv 1, 3 \pmod{6}$. These necessary conditions have been proven to be sufficient:

Theorem

$$\exists STS(v) \iff v \equiv 1,3 \pmod{6}$$

So, there exists an STS(v) for $v = 1, 3, 7, 9, 13, 15, 19, 21, 25, 17, 31, 33, \ldots$

A partial Steiner triple system consists of a set of triples \mathcal{B} with each pair of points appearing in at most one $B_i \in \mathcal{B}$. Then, we can formulate the search problem as follows.

Design Strategies for Heuristic Algorithms 00 000000 00000 Heuristic Searches Applied to Various Problems

Hill-climbing Algorithms

Searching for Steiner Triple Systems

```
PROBLEM: CONSTRUCT A STEINER TRIPLE SYSTEM
INSTANCE: v such that v \equiv 1, 3 \pmod{6}
Find: Maximize |\mathcal{B}|
subject to: ([1, v], \mathcal{B}) is a
partial Steiner triple system
```

The **universe** \mathcal{X} is the set of all sets of blocks \mathcal{B} , such that $([1, v], \mathcal{B})$ is a partial Steiner triple system.

An **optimal solution** is any feasible solution with $|\mathcal{B}| = \frac{v(v-1)}{6}$.

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Hill-climbing Algorithms

Stinson's hill-climbing algorithm for STSs

```
Algorithm Stinson's Algorithm(v)

Numblocks \leftarrow 0

V \leftarrow \{1, 2, \dots v\}

\mathcal{B} \leftarrow \emptyset

While (Numblocks < \frac{v(v-1)}{2}) do { SWITCH}

output (V, \mathcal{B})
```

To present SWITCH, we need:

Definition

A point x is said to be a live point in ([1, v], B) if $r_x < \frac{v-1}{2}$. A pair $\{x, y\}$ is said to be a live pair in ([1, v], B) if there exists no $B \in B$ with $\{x, y\} \subseteq B$

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Design Strategies for Heuristic Algorithms DO DO DOOOOO DOOOO Heuristic Searches Applied to Various Problems

Hill-climbing Algorithms

Stinson's hill-climbing for STSs: Switch Algorithm

Algorithm SWITCH

Chosse a random live point x. Choose random y, z such that $\{x, y\}$ and $\{x, z\}$ are live pairs. If $(\{y, z\}$ is a live pair) then $\mathcal{B} \leftarrow \mathcal{B} \cup \{\{x, y, z\}\}$ Numblocks \leftarrow Numblocks +1 else Let $\{w, y, z\} \in \mathcal{B}$ be the block containing $\{y, z\}$

Let
$$\{w, y, z\} \in \mathcal{B}$$
 be the block containing $\{y, z \in \mathcal{B} \cup \{x, y, z\}\} \setminus \{\{w, y, z\}\}$

See implementation details in the textbook.

Using appropriatte data structures, SWITCH is implemented in constant time. $\langle \Box \rangle \langle \partial \rangle \langle \Xi \rangle \langle \Xi \rangle \langle \Xi \rangle \langle \Xi \rangle$

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Two heuristics for the Knapsack Problem

```
Knapsack (Optimization) Problem
```

```
Instance: Profits p_0, p_1, \ldots, p_{n-1}
Weights w_0, w_1, \ldots, w_{n-1}
Knapsack capacity M
```

Universe:
$$\mathcal{X} = \{0, 1\}^n$$
 (set of all *n*-tuples)
an *n*-tuple $[x_0, x_1, \dots, x_{n-1}]$ is feasible if
 $\sum_{i=0}^{n-1} w_i x_i \leq M.$

Objective: maximize $P(X) = \sum_{i=0}^{n-1} p_i x_i$.

Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Algorithm KNAPSACKSIMULATEDANNEALING(
$$c_{max}, T_0, \alpha$$
)
 $c \leftarrow 0; T \leftarrow T_0; X \leftarrow [x_0, x_1, \dots, x_{n-1}] = [0, 0, \dots, 0];$
 $CurW \leftarrow 0; X_{best} \leftarrow X;$
while $(c \leq c_{max})$ do
 $j \leftarrow randomInt(0, n - 1); Y \leftarrow X; y_j \leftarrow 1 - x_j;$ (using $N_1(X)$)
if $(y_j = 1)$ and $(curW + w_j > M)$ then $Y \leftarrow fail;$
if $(Y \neq fail)$ then if $(y_{j}=1)$ then
 $X \leftarrow Y;$
 $curW \leftarrow curW + w_j;$
if $P(X) > P(X_{best})$ then $X_{best} \leftarrow X;$
else $r \leftarrow random(0, 1);$
if $(r < e^{-p_j/T})$ then
 $X \leftarrow Y;$ $curW \leftarrow curW - w_j;$
 $c \leftarrow c + 1; T \leftarrow \alpha T;$
return $(X_{best});$

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Knapsack Simulated Annealing Results

TABLE 5.3 Summary data for the knapsack simulated annealing algorithm.

α .	Cmax	profits found		
		minimum	maximum	average
0.999	1000	1441	1454	1446.8
0.999	5000	1448	1456	1452.1
0.999	20000	1448	1456	1450.9
0.9995	1000	1445	1455	1448.4
0.9995	5000	1450	1458	1454.6
0.9995	20000	1452	1458	1453.9
0.9999	1000	1445	1455	1449.6
0.9999	5000	1450	1458	1454.3
0.9999	20000	1453	1458	1456.1

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Heuristic Search Intro 00 00000 00	Design Strategies for Heuristic Algorithms 00 000000 000000	Heuristic Searches Applied to Various Problems

Tabu Search for Knapsack

We will use the same neighbourhood $N_1(.)$.

Do exhaustive search on the neighbourhood in order to find the best way to update the current solution.

Instead of Profit improvement only, we look for improvements based on the ratio $p_i/w_i\!\!:$

- Chose *i* with maximum p_i/w_i among the indexes *j* where $x_j = 0$, *j* is not on TABULIST, and changing x_j to 1 does not exceed *M*.
- ② If there is no j as above, then choose i with minimum p_i/w_i among the indexes j where $x_j = 1$ and j is not on TABULIST.

This can be expressed by saying that we want to maximize

$$(-1)^{x_j}\frac{p_j}{w_j}.$$

Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Algorithm KNAPSACKTABUSEARCH (c_{max}, L) Select a random feasible $X = [x_0, x_1, ..., x_{n-1}] \in \{0, 1\}^n$; $curW \leftarrow \sum_{i=0}^{n-1} x_i w_i; X_{best} \leftarrow X;$ for $(c \leftarrow 1; c < c_{max}; c \leftarrow c+1)$ do $N \leftarrow \{0, 1, \ldots, n-1\} \setminus \{j : j \text{ is in TABULIST}\};$ for each $(i \in N)$ do if $(x_i = 0)$ and $(curW + w_i > M)$ then $N \leftarrow N \setminus \{i\}$; if $(N = \emptyset)$ then break for-loop; Find $i \in N$ such that $(-1)^{x_i} p_i / w_i$ is maximum; TABULIST.INSERT(i, L); (removing oldest, if has L + 1 items) $x_i \leftarrow 1 - x_i$; (swap *i* coordinate) if $(x_i = 1)$ then $curW \leftarrow curW + w_i$; else $curW \leftarrow curW - w_i$: if $P(X) > P(X_{best})$ then $X_{best} \leftarrow X$; return X_{hest} :

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Heuristic Search Intro	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Two heuristics for the Kna	psack Problem	

average

13388643.5

13415747.5

13456205.2

13446933.8

13458145.8

13427333.6

13462902.4

13497932.2

optimal solutions found

Summary data for the knapsack tabu search algorithm (24 items).

profits found (in 25 runs)

maximum

Heuristic Search

TABLE 5.6

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minimum

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Heuristic Search Intro E 00 00 00000 00 00 00	Design Strategies for Heuristic Algorithms DO DO DODOOO DODOOO	Heuristic Searches Applied to Various Problems

A Genetic Algorithm for TSP

A Genetic Algorithm for the TSP

```
Traveling Salesman Problem (TSP)
```

Instance: a complete graph K_n a cost function $c: V \times V \to R$

Find: a Hamiltonian circuit $[x_0, x_1, \dots, x_{n-1}]$ that minimizes $C(X) = c(x_0, x_1) + c(x_1, x_2) + \dots + c(x_{n-1}, x_0)$

Note that 2n permutations represent the same cycle. Universe: $\mathcal{X} = \text{set of all } n!$ permutations. Steps:

- Selection of initial population.
- Mutation: steepest ascent 2-opt.
- Recombination using two methods: partially matched crossover and another method.

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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Mutation

Steepest ascent algorithm based on the 2-opt heuristic:



Gain in applying a 2-opt move:

$$G(X, i, j) = C(X) - C(X_{ij})$$

= $c(x_i, x_{i+1}) + c(x_j, x_{j+1}) - c(x_{i+1}, x_{j+1}) - c(x_i, x_j)$

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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N(X) =all $Y \in \mathcal{X}$ that can be obtained from X by a 2-opt move.

```
Algorithm STEEPESTASCENTTWOOPT(X)
              done \leftarrow false:
              while (not done) do
                      done \leftarrow true; q_0 \leftarrow 0;
                      for i \leftarrow 0 to n-1 do
                          for j \leftarrow i+2 to n-1 do
                               q \leftarrow G(X, i, j);
                               if (q > q_0) then
                                  q_0 \leftarrow q; i_0 \leftarrow i; j_0 \leftarrow j;
                      if (g_0 > 0) then
                        X \leftarrow X_{i_0, i_0};
                         done \leftarrow false:
```

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Design Strategies for Heuristic Algorithms DO DO DODODO DODOO DODOO Heuristic Searches Applied to Various Problems

A Genetic Algorithm for TSP

Selecting the initial population

Randomly pick one and then mutate it:

```
Algorithm SELECT(popsize)
for i \leftarrow 0 to popsize - 1 do
r \leftarrow \text{RANDOMINTEGER}(0, n! - 1);
P_i \leftarrow \text{PERMLEXUNRANK}(n, r);
STEEPESTASCENTTWOOPT(P_i);
return [P_0, P_1, \dots, P_{popsize-1}];
```

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Design Strategies for Heuristic Algorithms 00 00000 00000 Heuristic Searches Applied to Various Problems

A Genetic Algorithm for TSP

Recombination algorithm 1: Partially Matched Crossover

Algorithm PMRec(A, B)

 $h \leftarrow \text{RANDOMINTEGER}(10, n/2)$; (length of the substring)

 $j \leftarrow \text{RANDOMINTEGER}(0, n-1)$; (start of the substring)

 $(C, D) \leftarrow \text{PARTIALLYMATCHEDCROSSOVER}(A, B, j, (h+j)mod n)$ STEEPESTASCENTTWOOPT(C);

STEEPESTASCENTTWOOPT(D);

return (C, D);

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A Genetic Algorithm for TSP

Recombination Algorithm 2

Algorithm MGKRec(A, B)

 $h \leftarrow \text{RANDOMINTEGER}(10, n/2)$; (length of the substring)

 $j \leftarrow \text{RANDOMINTEGER}(0, n-1)$; (start of the substring) $T \leftarrow \emptyset$;

(pick subcycle of length h starting from pos j:)

for
$$i \leftarrow 0$$
 to $h - 1$ do

 $D[i] \leftarrow B[(i+j) \mod n];$

 $T \leftarrow T \cup \{D[i]\};$

Complete cycle with permutation in ${\cal A}$ using guys not already in ${\cal D}$ in the order prescribed by ${\cal A}$:

for $j \leftarrow 0$ to n-1 do

if $A[j] \notin T$ then $\{D[i] \leftarrow A[j]; i \leftarrow i+1; \}$ STEEPESTASCENTTWOOPT(D);

	Design Strategies for Heuristic Algorithms	Heuristic Searches Applied to Various Problems
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(Algorithm continued)
     (Similarly build C swapping A and B roles:)...
     j \leftarrow \text{RANDOMINTEGER}(0, n-1); (start of the substring)
     T \leftarrow \emptyset:
     for i \leftarrow 0 to h - 1 do
         C[i] \leftarrow A[(i+j) \mod n];
         T \leftarrow T \cup \{C[i]\}:
     for i \leftarrow 0 to n-1 do
         if B[j] \notin T then \{C[i] \leftarrow B[j]; i \leftarrow i+1; \}
     STEEPESTASCENTTWOOPT(C);
     return (C, D);
```
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Design Strategies for Heuristic Algorithms 00 000000 000000 Heuristic Searches Applied to Various Problems

A Genetic Algorithm for TSP

Genetic Algorithm for TSP

```
Algorithm GENETICTSP(popsize, c_{max})
      [P_0, P_1, \ldots, P_{nonsize-1}] \leftarrow \text{SELECT}(popsize);
     Sort P_0, P_1, \ldots, P_{popsize-1} in increasing order of cost.
     X_{best} \leftarrow P_0; BestCost \leftarrow C(P_0);
      for (c \leftarrow 1; c < c_{max}; c \leftarrow c+1) do
          for i \leftarrow 0 to popsize/2 - 1 do
               (P_{ponsize+2i}, P_{ponsize+2i+1}) \leftarrow \text{Rec} (P_{2i}, P_{2i+1});
          Sort P_0, P_1, \ldots, P_{2popsize-1} in increasing order of cost.
          curCost \leftarrow C(P_0):
          if (curCost < BestCost) then
             X_{best} \leftarrow P_0;
             BestCost \leftarrow curCost:
      return X_{hest}:
```

Design Strategies for Heuristic Algorithms 00 000000 Heuristic Searches Applied to Various Problems

A Genetic Algorithm for TSF

						cost for	ind	
М	n	Opt. Cost	popsize	Cmax	min	max	avg	No. Opt. found
M50a	50	185	8	50	192	214	200.50	0
				100	191	219	200.00	0
				200	190	203	196.60	0
			16	50	187	207	193.20	0
				100	187	206	193.20	0
				200	187	200	193.70	0
			32	50	189	205	194.70	0
				100	186	199	190.70	0
				200	188	200	192.40	0
M50b	50	158	8	50	163	184	175.40	0
				100	163	195	173.70	0
				200	160	191	177.30	0
			16	50	159	176	167.40	0
				100	163	184	171.50	0
				200	161	189	172.10	0
			32	50	161	173	167.60	0
				100	163	178	169.40	0
				200	159	178	166.70	0
M50c	50	155	8	50	162	181	169.40	0
				100	159	186	169.50	0
				200	159	187	169.30	0
			16	50	155	171	161.30	1
				100	155	182	166.10	1
				200	157	182	167.70	0
			32	50	155	170	161.60	1
				100	158	167	161.40	0
				200	157	180	162.50	0

TABLE 5.7 GENETICTSP data with recombination operation PMREC.

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Heuristic Search Intro 00 00000 00 Design Strategies for Heuristic Algorithms 00 00 000000 Heuristic Searches Applied to Various Problems

A Genetic Algorithm for TSF

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TABLE 5.8		
GENETICTSP	with recombination operation	MGKREC.

10000					cost found			
M	n	Opt. Cost	popsize	Cmaz	min	max	avg	No. Opt. found
M50a	50	185	8	50	186	196	191.70	0
brad				100	186	199	190.30	0
marth				200	186	194	189.20	0
1.1.1			16	50	186	192	189.20	0
				100	185	192	187.00	3
10.01				200	185	192	187.60	1
1161 120	1		32	50	186	192	188.10	0
				100	185	190	187.30	1
				200	185	190	187.30	1
M50b	50	158	8	50	160	171	165.30	0
				100	159	166	161.60	0
1000000				200	159	170	162.00	0
新新新 市。			16	50	158	164	161.20	1
				100	158	162	159.80	1
	12			200	159	163	160.70	0
			32	50	158	165	160.70	1
				100	159	163	160.30	0
				200	158	160	158.90	2
M50c	50	155	8	50	156	168	160.50	0
				100	155	167	160.70	2
				200	155	162	157.30	5
			16	50	155	162	157.50	2
				100	155	159	156.30	5
				200	155	159	155.70	8
	8		32	50	155	159	156.10	6
	1.0			100	155	158	155.40	8
				200	155	156	155.10	9

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