Optimization Techniques

Genetic Algorithms

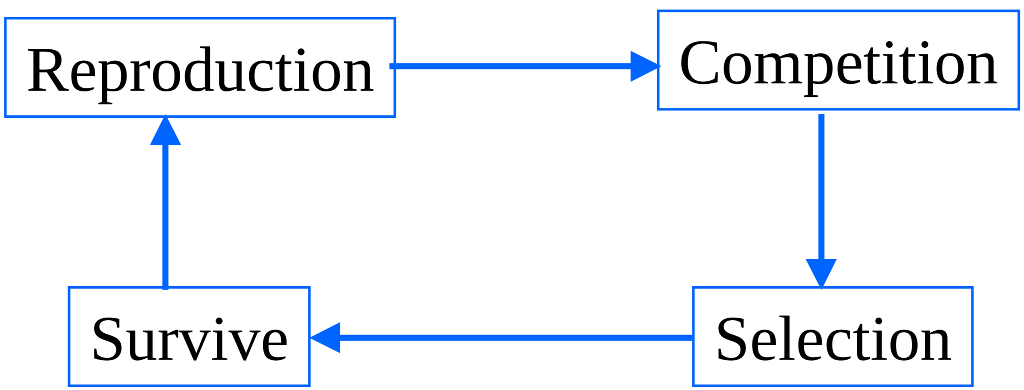
And other approaches for similar applications

Optimization Techniques

- Mathematical Programming
- Network Analysis
- Branch & Bound
- Genetic Algorithm
- Simulated Annealing
- Tabu Search

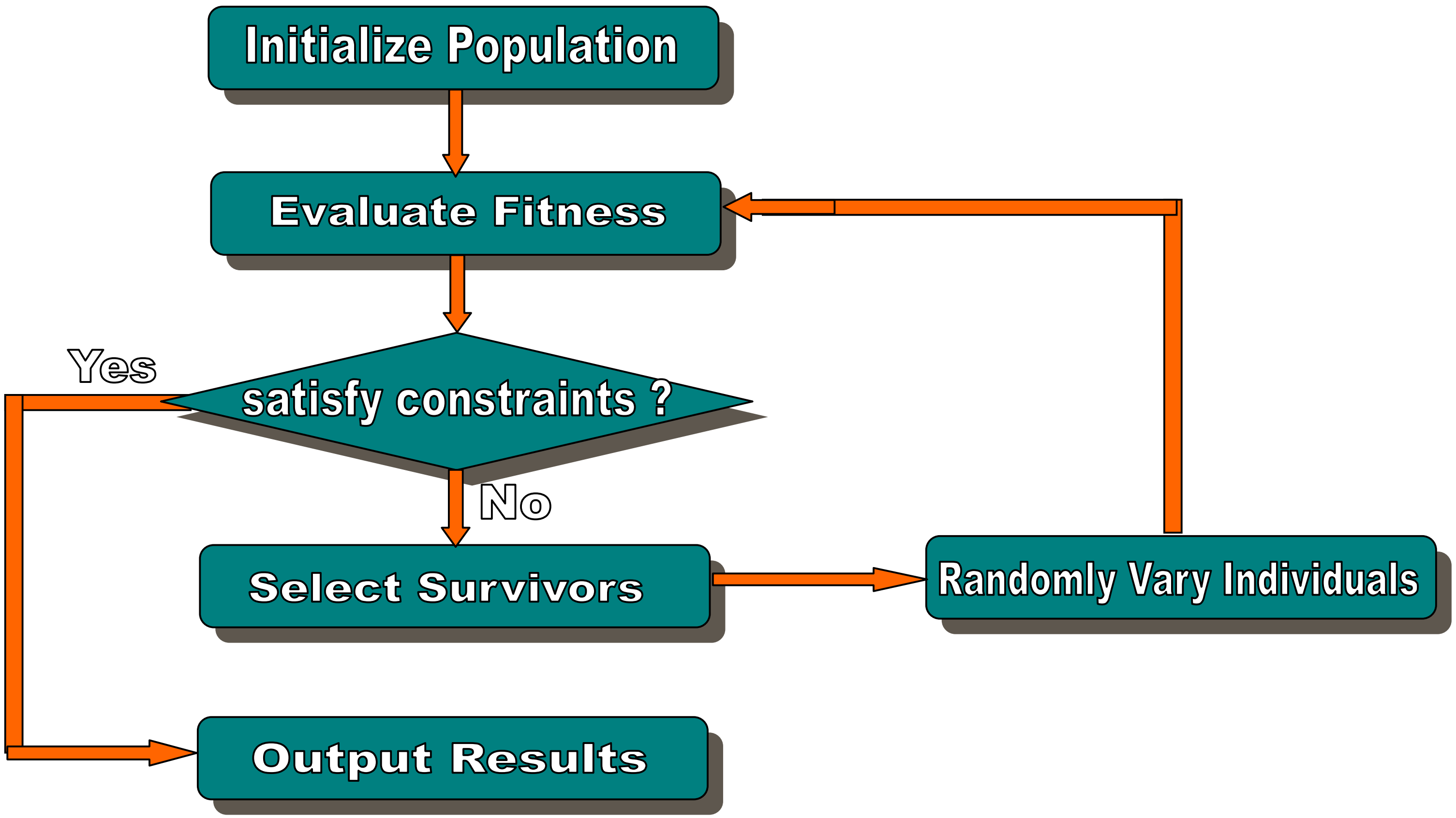
Genetic Algorithm

- Based on Darwinian Paradigm



- Intrinsically a robust search and optimization mechanism

Conceptual Algorithm



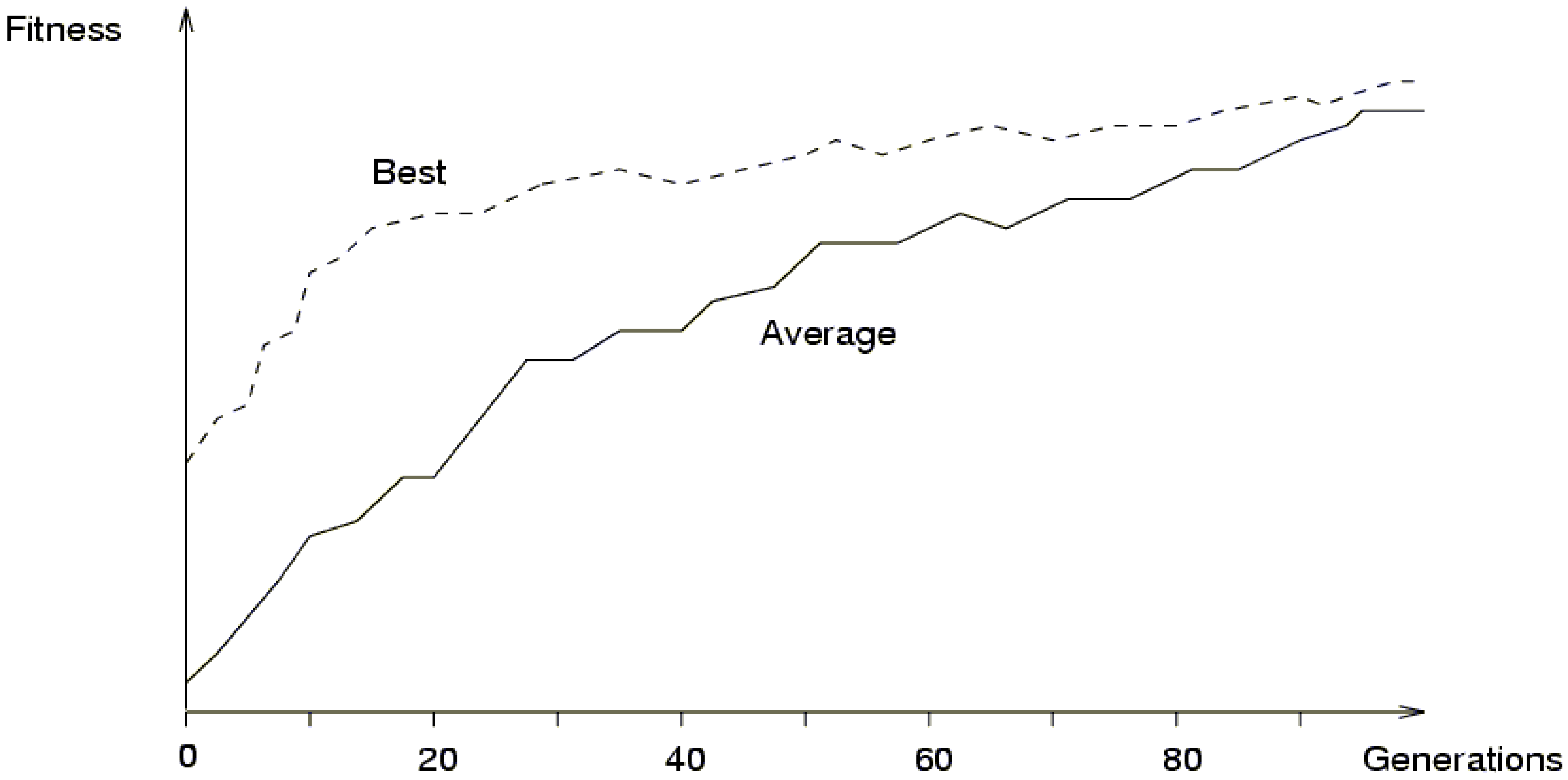
Genetic Algorithm Introduction 1

- Inspired by natural evolution
- Population of individuals
  - Individual is feasible solution to problem
- Each individual is characterized by a Fitness function
  - Higher fitness is better solution
- Based on their fitness, parents are selected to reproduce offspring for a new generation
  - Fitter individuals have more chance to reproduce
  - New generation has same size as old generation; old generation dies
- Offspring has combination of properties of two parents
- If well designed, population will converge to optimal solution

Algorithm

```
BEGIN
  Generate initial population;
  Compute fitness of each individual;
  REPEAT /* New generation /*
    FOR population_size / 2 DO
      Select two parents from old generation;
       /* biased to the fitter ones */
      Recombine parents for two offspring;
      Compute fitness of offspring;
      Insert offspring in new generation
    END FOR
  UNTIL population has converged
END
```

Example of convergence



Introduction 2

- Reproduction mechanisms have no knowledge of the problem to be solved

- Link between genetic algorithm and problem:
  - Coding
  - Fitness function

Basic principles 1

- Coding or Representation
  - String with all parameters
- Fitness function
  - Parent selection
- Reproduction
  - Crossover
  - Mutation
- Convergence
  - When to stop

Basic principles 2

- An individual is characterized by a set of parameters: Genes
- The genes are joined into a string: Chromosome

- The chromosome forms the genotype
- The genotype contains all information to construct an organism: the phenotype

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- Reproduction is a “dumb” process on the chromosome of the genotype
- Fitness is measured in the real world (‘struggle for life’) of the phenotype

Coding

- Parameters of the solution (genes) are concatenated to form a string (chromosome)
- All kind of alphabets can be used for a chromosome (numbers, characters), but generally a binary alphabet is used
- Order of genes on chromosome can be important
- Generally many different codings for the parameters of a solution are possible
- Good coding is probably the most important factor for the performance of a GA
- In many cases many possible chromosomes do not code for feasible solutions

Genetic Algorithm

- Encoding
- Fitness Evaluation
- Reproduction
- Survivor Selection

Encoding

- Design alternative → individual (chromosome)
- Single design choice → gene
- Design objectives → fitness

Example

- Problem
  - Schedule *n* jobs on *m* processors such that the maximum span is minimized.

Design alternative: job i (i=1,2,…n) is assigned to processor j (j=1,2,…,m)

Individual: A n-vector **x** such that $x_i = 1, \ldots, or\ m$

Design objective: minimize the maximal span

Fitness: the maximal span for each processor

Reproduction

- Reproduction operators
  - Crossover
  - Mutation

Reproduction

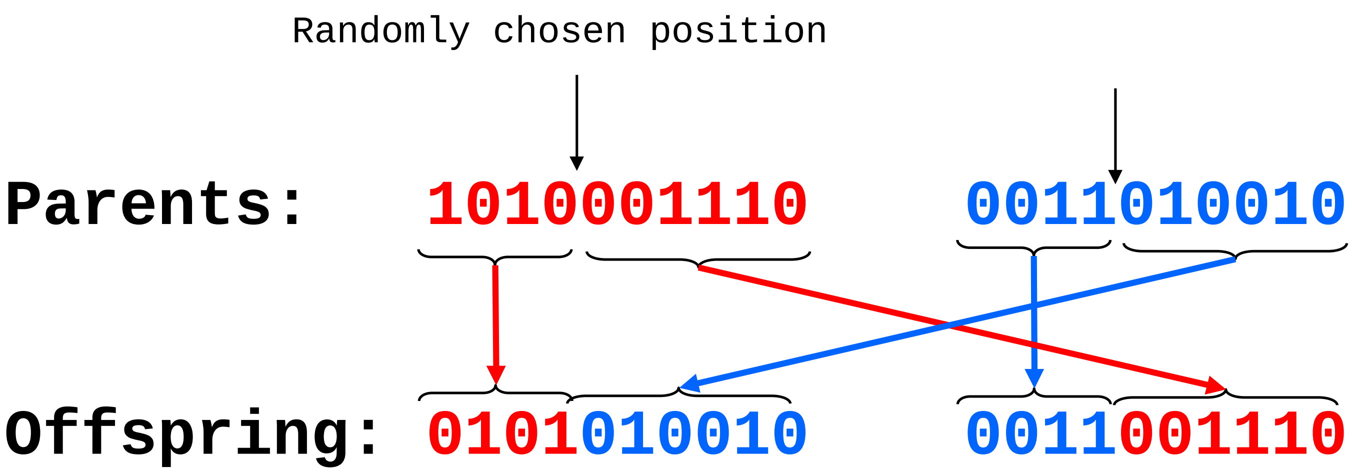
- Crossover
  - Two parents produce two offspring
  - There is a chance that the chromosomes of the two parents are copied unmodified as offspring
  - There is a chance that the chromosomes of the two parents are randomly recombined (crossover) to form offspring
  - Generally the chance of crossover is between 0.6 and 1.0
- Mutation
  - There is a chance that a gene of a child is changed randomly
  - Generally the chance of mutation is low (e.g. 0.001)

Reproduction Operators

- Crossover
  - Generating offspring from two selected parents
    - Single point crossover
    - Two point crossover (Multi point crossover)
    - Uniform crossover

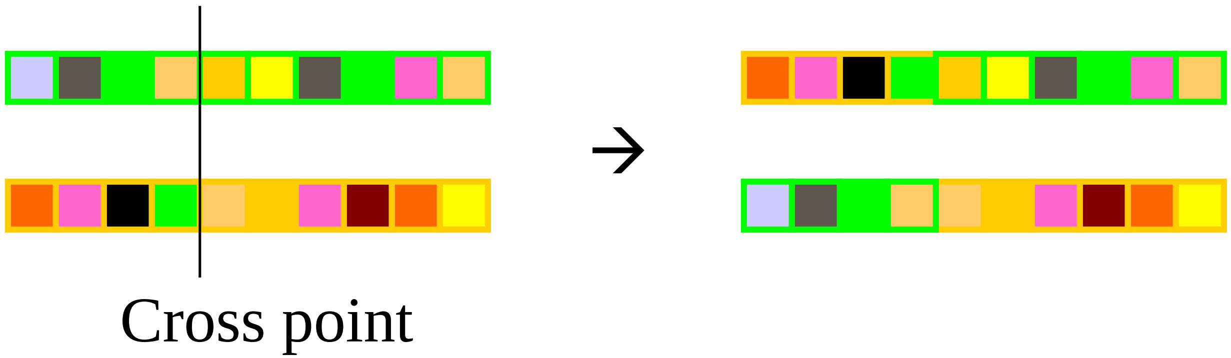
One-point crossover 1

- Randomly one position in the chromosomes is chosen
- Child 1 is head of chromosome of parent 1 with tail of chromosome of parent 2
- Child 2 is head of 2 with tail of 1

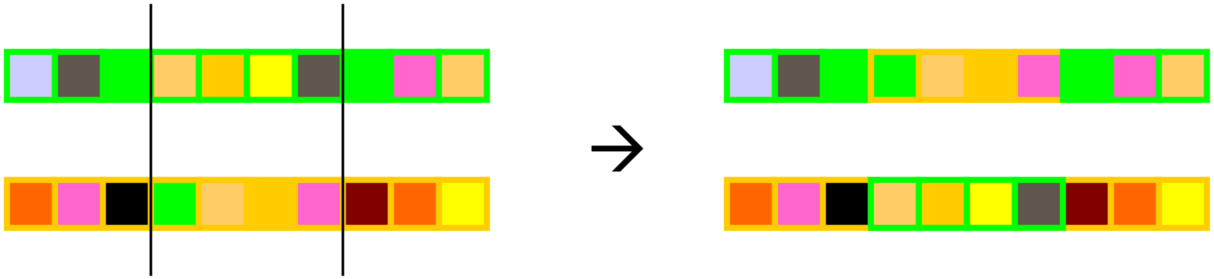


Reproduction Operators comparison

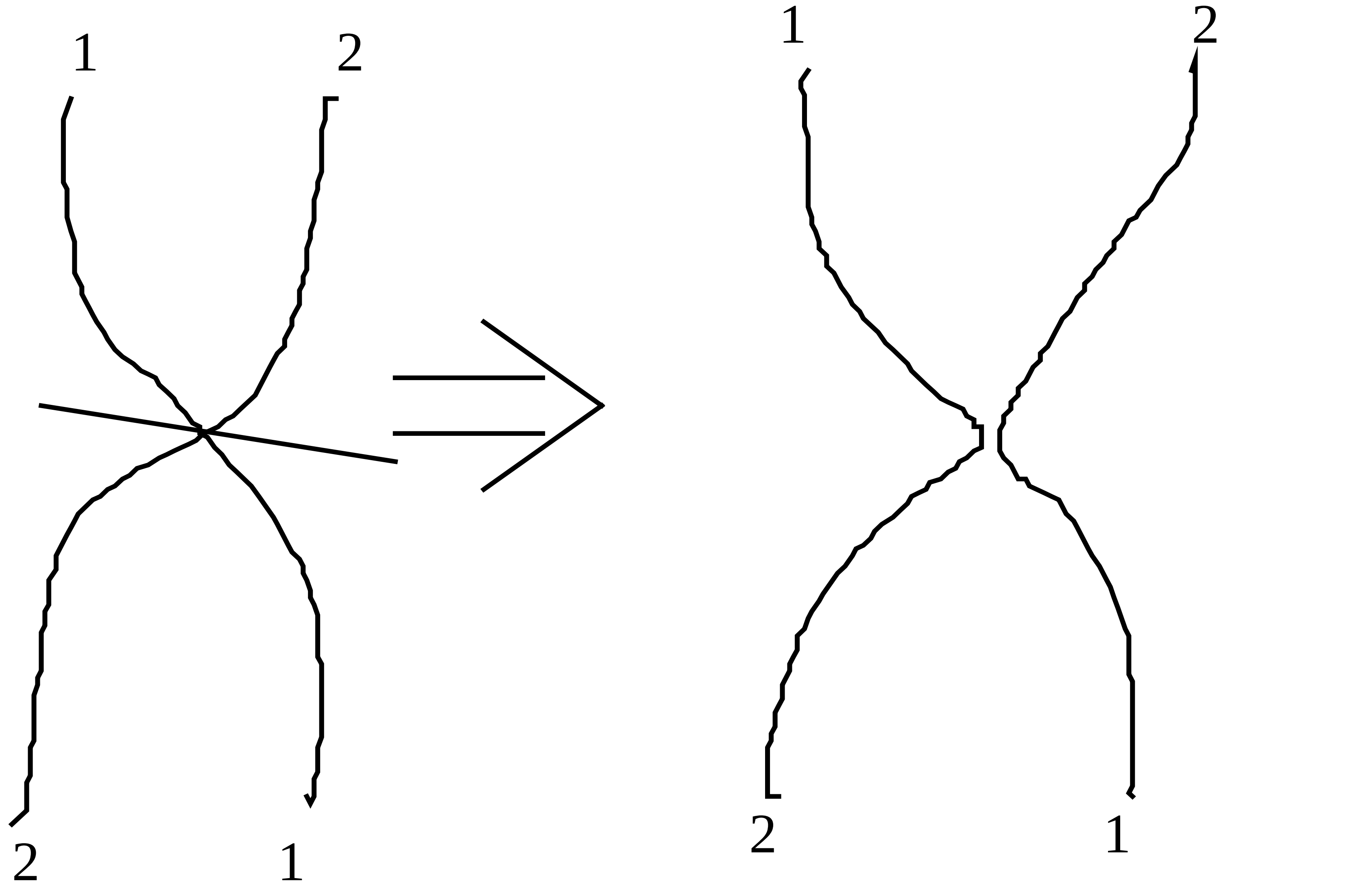
- Single point crossover



- Two point crossover (Multi point crossover)

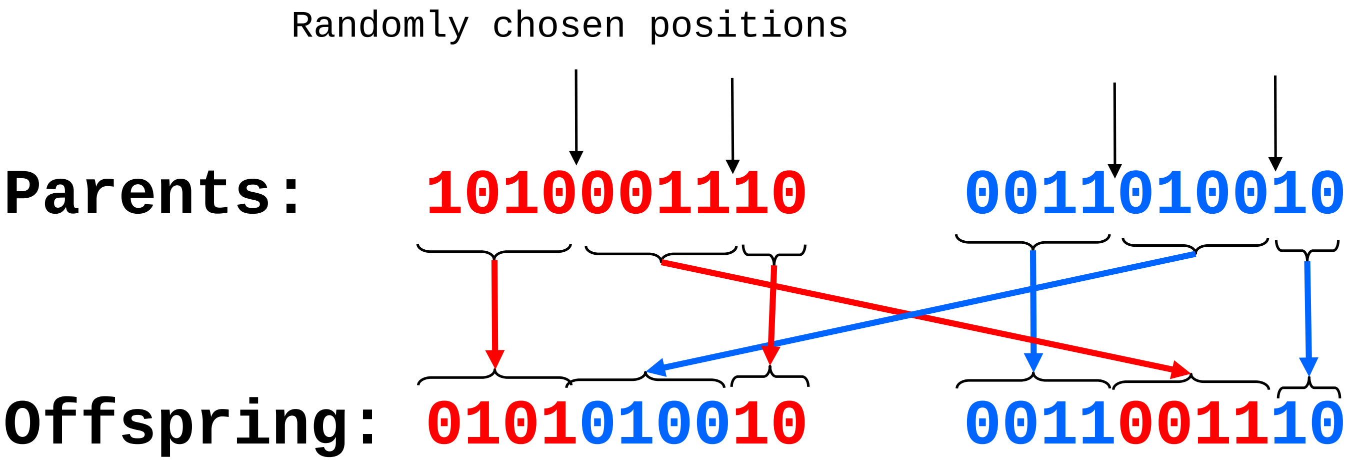


One-point crossover - Nature



Two-point crossover

- Randomly two positions in the chromosomes are chosen
- Avoids that genes at the head and genes at the tail of a chromosome are always split when recombined



Uniform crossover

- A random mask is generated
- The mask determines which bits are copied from one parent and which from the other parent
- Bit density in mask determines how much material is taken from the other parent (takeover parameter)

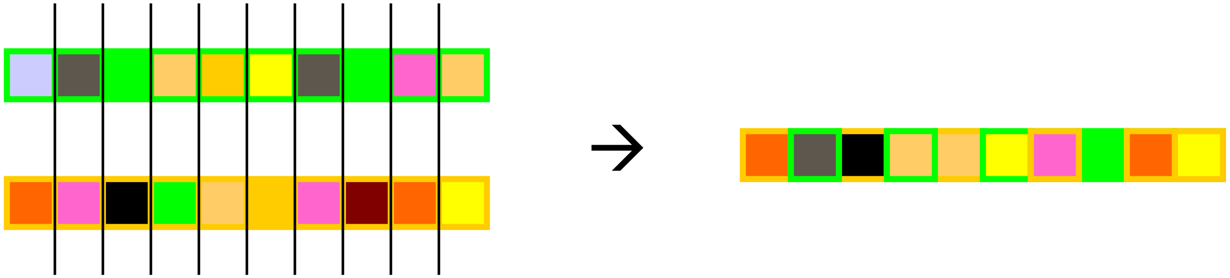
```
Mask:       0110011000    (Randomly generated)

Parents:    1010001110    0011010010


Offspring:  0011001010    1010010110
```

Reproduction Operators

- Uniform crossover



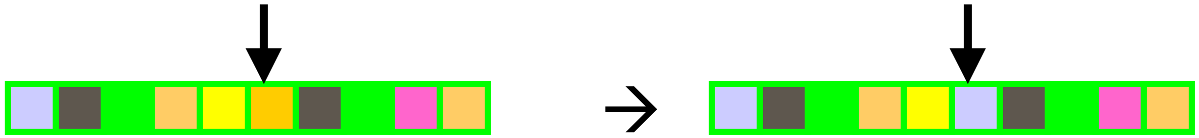
- Is uniform crossover better than single crossover point?
  - Trade off between
    - Exploration: introduction of new combination of features
    - Exploitation: keep the good features in the existing solution

Problems with crossover

- Depending on coding, simple crossovers can have high chance to produce illegal offspring
  - E.g. in TSP with simple binary or path coding, most offspring will be illegal because not all cities will be in the offspring and some cities will be there more than once
- Uniform crossover can often be modified to avoid this problem
  - E.g. in TSP with simple path coding:
    - Where mask is 1, copy cities from one parent
    - Where mask is 0, choose the remaining cities in the order of the other parent

Reproduction Operators

- Mutation
  - Generating new offspring from single parent



  - Maintaining the diversity of the individuals
    - Crossover can only explore the combinations of the current gene pool
    - Mutation can “generate” new genes

Reproduction Operators

- Control parameters: **population size, crossover / mutation probability**
  - Problem specific
  - Increase population size
    - Increase diversity and computation time for each generation
  - Increase crossover probability
    - Increase the opportunity for recombination but also disruption of good combination
  - Increase mutation probability
    - Closer to randomly search
    - Help to introduce new gene or reintroduce the lost gene
- Varies the population
  - Usually using crossover operators to recombine the genes to generate the new population, then using mutation operators on the new population

Parent/Survivor Selection

- Strategies
  - Survivor selection
    - Always keep the best one
    - Elitist: deletion of the K worst
    - Probability selection : inverse to their fitness
    - Etc.

Parent/Survivor Selection

- Too strong fitness selection bias can lead to sub-optimal solution
- Too little fitness bias selection results in unfocused and meandering search

Parent selection

Chance to be selected as parent proportional to fitness

- Roulette wheel

To avoid problems with fitness function

- Tournament

Not a very important parameter

Parent/Survivor Selection

- Strategies
  - Parent selection
    - Uniform randomly selection
    - Probability selection : proportional to their fitness
    - Tournament selection (Multiple Objectives)
      - Build a small comparison set
      - Randomly select a pair with the higher rank one beats the lower one
        - Non-dominated one beat the dominated one
        - **Niche count**: the number of points in the population within certain distance, higher the niche count, lower the rank.
    - Etc.

Others

- Global Optimal
- Parameter Tuning
- Parallelism
- Random number generators

Example of coding for TSP

Travelling Salesman Problem

- Binary
  - Cities are binary coded; chromosome is string of bits
    - Most chromosomes code for illegal tour
    - Several chromosomes code for the same tour
- Path
  - Cities are numbered; chromosome is string of integers
    - Most chromosomes code for illegal tour
    - Several chromosomes code for the same tour
- Ordinal
  - Cities are numbered, but code is complex
  - All possible chromosomes are legal and only one chromosome for each tour
- Several others

Roulette wheel

- Sum the fitness of all chromosomes, call it T
- Generate a random number N between 1 and T
- Return chromosome whose fitness added to the running total is equal to or larger than N
- Chance to be selected is exactly proportional to fitness

Chromosome:	**1**	**2**	**3**	**4**	**5**	**6**
Fitness:	**8**	**2**	**17**	**7**	**4**	**11**
Running total:	**8**	**10**	**27**	**34**	**38**	**49**
N ($1 \leq N \leq 49$):			**23**			
Selected:			**3**			

Tournament

- Binary tournament
  - Two individuals are randomly chosen; the fitter of the two is selected as a parent
- Probabilistic binary tournament
  - Two individuals are randomly chosen; with a chance p, $0.5<p<1$, the fitter of the two is selected as a parent
- Larger tournaments
  - n individuals are randomly chosen; the fittest one is selected as a parent

- By changing n and/or p, the GA can be adjusted dynamically

Problems with fitness range

- Premature convergence
  - ΔFitness too large
  - Relatively superfit individuals dominate population
  - Population converges to a local maximum
  - Too much exploitation; too few exploration
- Slow finishing
  - ΔFitness too small
  - No selection pressure
  - After many generations, average fitness has converged, but no global maximum is found; not sufficient difference between best and average fitness
  - Too few exploitation; too much exploration

Solutions for these problems

- Use tournament selection
  - Implicit fitness remapping
- Adjust fitness function for roulette wheel
  - Explicit fitness remapping
    - Fitness scaling
    - Fitness windowing
    - Fitness ranking

Will be explained below

Fitness Function

Purpose

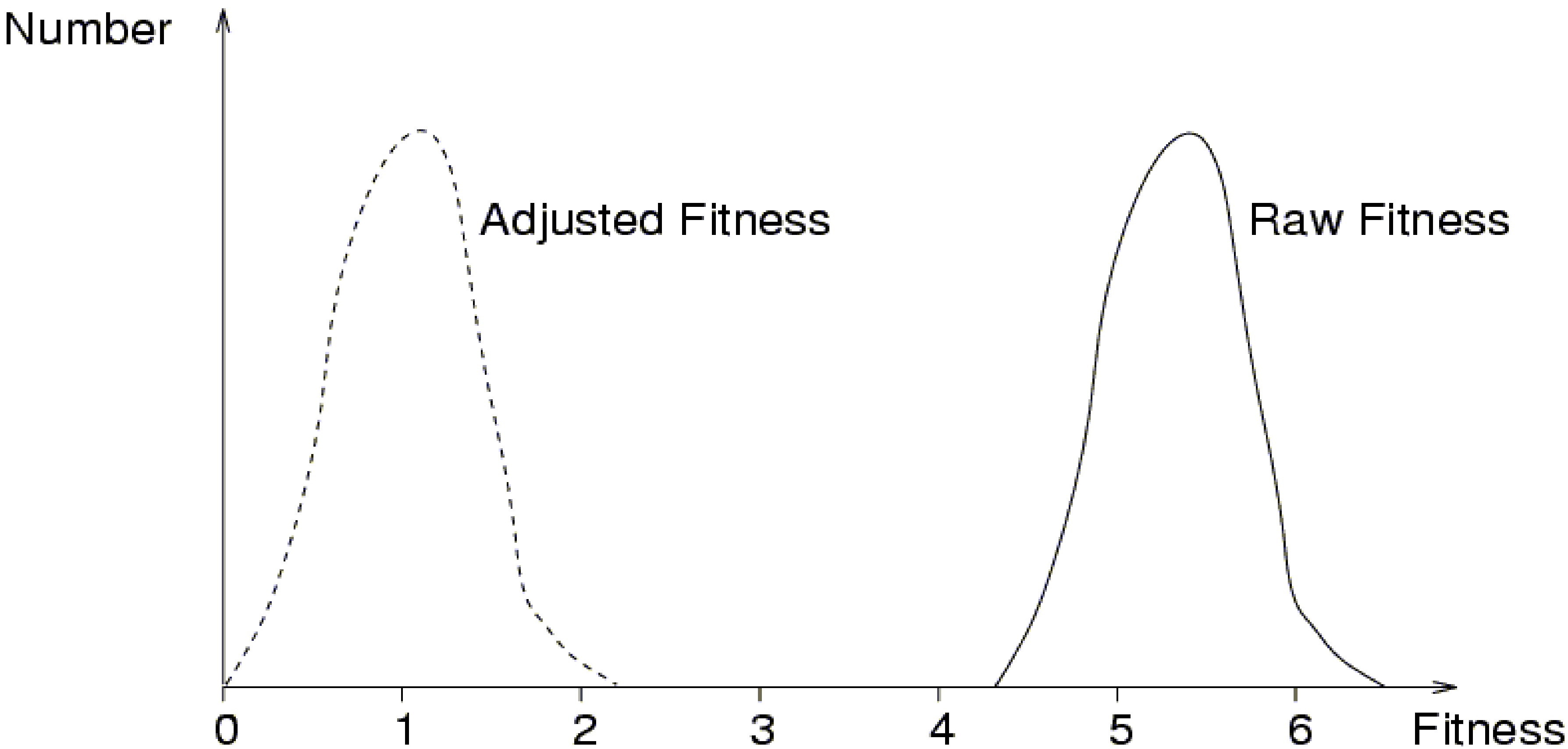
- Parent selection
- Measure for convergence
- For Steady state: Selection of individuals to die

- Should reflect the value of the chromosome in some “real” way
- Next to coding the most critical part of a GA

Fitness scaling

- Fitness values are scaled by subtraction and division so that worst value is close to 0 and the best value is close to a certain value, typically 2
  - Chance for the most fit individual is 2 times the average
  - Chance for the least fit individual is close to 0
- Problems when the original maximum is very extreme (super-fit) or when the original minimum is very extreme (super-unfit)
  - Can be solved by defining a minimum and/or a maximum value for the fitness

Example of Fitness Scaling



Fitness windowing

- Same as window scaling, except the amount subtracted is the minimum observed in the *n* previous generations, with *n* e.g. 10
- Same problems as with scaling

Fitness ranking

- Individuals are numbered in order of increasing fitness
- The rank in this order is the adjusted fitness
- Starting number and increment can be chosen in several ways and influence the results

- No problems with super-fit or super-unfit
- Often superior to scaling and windowing

Fitness Evaluation

- A key component in GA
- Time/quality trade off
- Multi-criterion fitness

Multi-Criterion Fitness

- Dominance and indifference
  - For an optimization problem with more than one objective function (f_i, $i=1,2,...n$)
  - given any two solution X_1 and X_2, then
    - X_1 dominates X_2 ($X_1 \succ X_2$), if

      $f_i(X_1) >= f_i(X_2)$, for all $i = 1,...,n$

    - X_1 is indifferent with X_2 ($X_1 \sim X_2$), if X_1 does not dominate X_2, and X_2 does not dominate X_1

Multi-Criterion Fitness

- Pareto Optimal Set
  - If there exists no solution in the search space which dominates any member in the set ***P***, then the solutions belonging the the set ***P*** constitute a global Pareto-optimal set.
  - Pareto optimal front
- Dominance Check

Multi-Criterion Fitness

- Weighted sum
  - $F(\boldsymbol{x}) = w_1 f_1(x_1) + w_2 f_2(x_2) + \ldots + w_n f_n(x_n)$
  - *Problems?*
    - *Convex and convex Pareto optimal front*

      Sensitive to the shape of the Pareto-optimal front
    - *Selection of weights?*

      Need some pre-knowledge

      Not reliable for problem involving uncertainties

Multi-Criterion Fitness

- Optimizing single objective
  - *Maximize:* $f_k(\mathbf{X})$

    Subject to:

    $f_i(\mathbf{X}) <= K_i, \quad i <> k$

    $\mathbf{X}$ *in F where F is the solution space.*

Multi-Criterion Fitness

- Weighted sum
  - *$F(\boldsymbol{x}) = w_1 f_1(x_1) + w_2 f_2(x_2) + \ldots + w_n f_n(x_n)$*
  - *Problems?*
    - *Convex and convex Pareto optimal front*

      Sensitive to the shape of the Pareto-optimal front
    - *Selection of weights?*

      Need some pre-knowledge

      Not reliable for problem involving uncertainties

Multi-Criterion Fitness

- Preference based weighted sum (**ISMAUT** ***Imprecisely Specific Multiple Attribute Utility Theory***)
  - $F(\boldsymbol{x}) = w_1 f_1(x_1) + w_2 f_2(x_2) + \ldots + w_n f_n(x_n)$
  - Preference
    - Given two know individuals **X** and **Y,** if we prefer **X** than **Y**, then

      $F(X) > F(Y),$

      that is

      $w_1(f_1(x_1)-f_1(y_1)) + \ldots + w_n(f_n(x_n)-f_n(y_n)) > 0$

Multi-Criterion Fitness

- All the preferences constitute a linear space ***$W_n = \{w_1, w_2, \ldots, w_n\}$***

  $w_1(f_1(x_1)-f_1(y_1)) + \ldots + w_n(f_n(x_n)-f_n(y_n)) > 0$

  $w_1(f_1(z_1)-f_1(p_1)) + \ldots + w_n(f_n(z_n)-f_n(p_n)) > 0$, *etc*

- For any two new individuals ***Y'*** and Y'', how to determine which one is more preferable?

Multi-Criterion Fitness

$$Min: \mu = \sum_k w_k [f_k(\mathbf{Y}') - f_k(\mathbf{Y}'')]$$

$$s.t.: \qquad W_n$$

$$Min: \mu' = \sum_k w_k [f_k(\mathbf{Y}'') - f_k(\mathbf{Y}')]$$

$$s.t.: \qquad W_n$$

Multi-Criterion Fitness

Then,

$$\mu > 0 \Rightarrow \mathbf{Y}' \succ \mathbf{Y}''$$

$$\mu' > 0 \Rightarrow \mathbf{Y}'' \succ \mathbf{Y}'$$

Otherwise,

$$\mathbf{Y}' \sim \mathbf{Y}''$$

Construct the dominant relationship among some indifferent ones according to the preferences.

Other parameters of GA 1

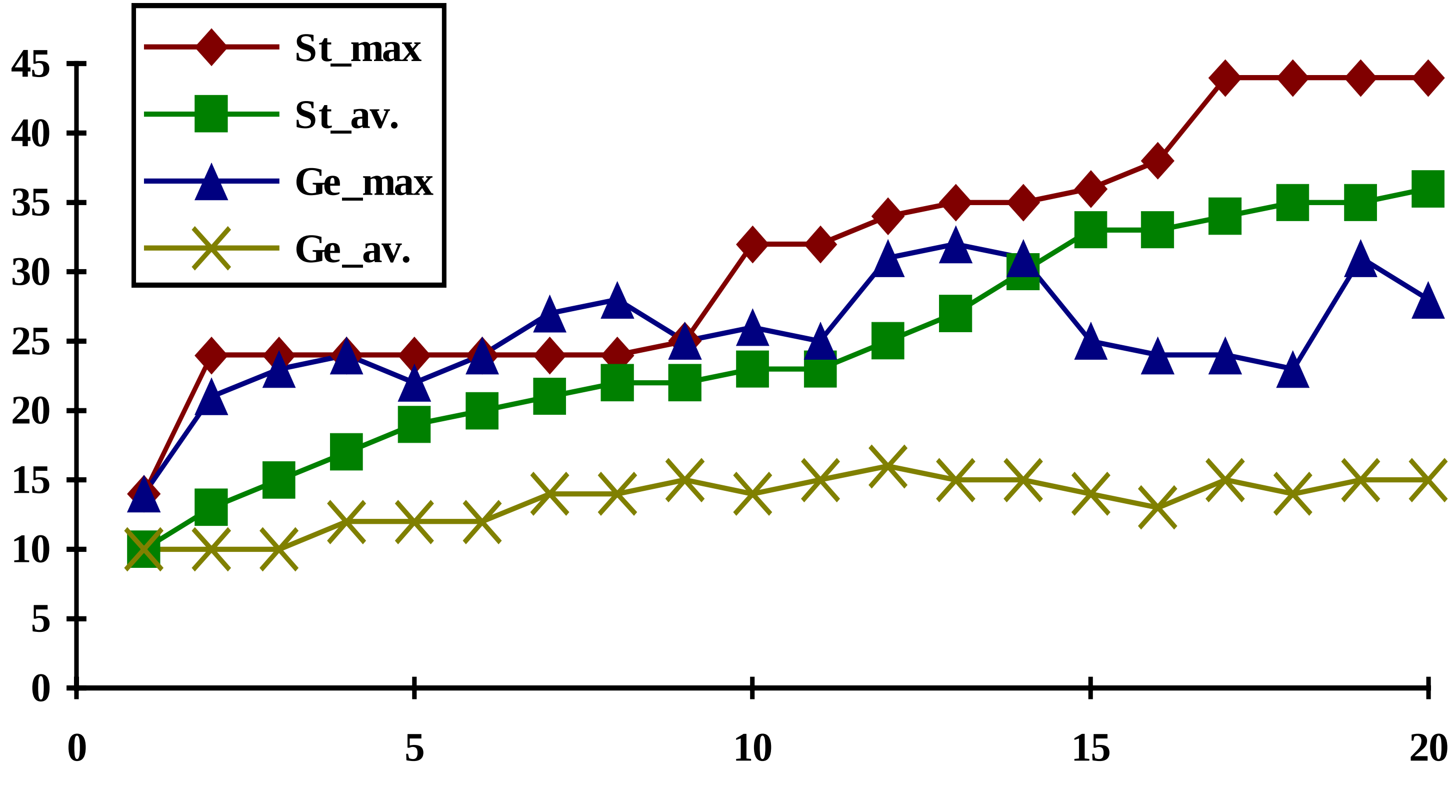
- Initialization:
  - Population size
  - Random
  - Dedicated greedy algorithm
- Reproduction:
  - Generational: as described before (insects)
  - Generational with elitism: fixed number of most fit individuals are copied unmodified into new generation
  - Steady state: two parents are selected to reproduce and two parents are selected to die; two offspring are immediately inserted in the pool (mammals)

Other parameters of GA 2

- Stop criterion:
  - Number of new chromosomes
  - Number of new and unique chromosomes
  - Number of generations
- Measure:
  - Best of population
  - Average of population
- Duplicates
  - Accept all duplicates
  - Avoid too many duplicates, because that degenerates the population (inteelt)
  - No duplicates at all

Example run

<u>Maxima</u> and <u>Averages</u> of steady state and generational replacement



Simulated Annealing

- What
  - Exploits an analogy between the annealing process and the search for the optimum in a more general system.

Annealing Process

- Annealing Process
  - Raising the temperature up to a very high level (melting temperature, for example), the atoms have a higher energy state and a high possibility to re-arrange the crystalline structure.
  - Cooling down slowly, the atoms have a lower and lower energy state and a smaller and smaller possibility to re-arrange the crystalline structure.

Simulated Annealing

- Analogy
  - Metal ←→ Problem
  - Energy State ←→ Cost Function
  - Temperature ←→ Control Parameter
  - A completely ordered crystalline structure ←→ the optimal solution for the problem

Global optimal solution can be achieved as long as the cooling process is slow enough.

Metropolis Loop

- The essential characteristic of simulated annealing
- Determining how to randomly explore new solution, reject or accept the new solution at a constant temperature T.
- Finished until equilibrium is achieved.

Metropolis Criterion

- Let
  - **X** be the current solution and **X'** be the new solution
  - $C(\mathbf{x})$ ($C(\mathbf{x'})$)be the energy state (cost) of **x** (**x'**)
- Probability $P_{accept} = \exp\left[(C(\mathbf{x})-C(\mathbf{x'}))/ T\right]$
- Let ***N=Random***(0,1)
- Unconditional accepted if
  - ***C(x') < C(x), the new solution is better***
- Probably accepted if
  - ***C(x') >= C(x), the new solution is worse . Accepted only when*** $N < P_{accept}$

Algorithm

Initialize initial solution **x** **,** highest temperature $\mathbf{T_h}$**,** and coolest temperature $\mathbf{T_l}$

$\mathbf{T = T_h}$

When the temperature is higher than $\mathbf{T_l}$

While not in equilibrium

Search for the new solution **X’**

Accept or reject **X’** according to Metropolis Criterion

End

Decrease the temperature **T**

End

Simulated Annealing

- Definition of solution
- Search mechanism, i.e. the definition of a neighborhood
- Cost-function

Control Parameters

- Definition of equilibrium
  - Cannot yield any significant improvement after certain number of loops
  - A constant number of loops
- Annealing schedule (i.e. How to reduce the temperature)
  - A constant value, $T' = T - T_d$
  - A constant scale factor, $T' = T * R_d$
    - A scale factor usually can achieve better performance

Control Parameters

- Temperature determination
  - Artificial, without physical significant
  - Initial temperature
    - 80-90% acceptance rate
  - Final temperature
    - A constant value, i.e., based on the total number of solutions searched
    - No improvement during the entire Metropolis loop
    - Acceptance rate falling below a given (small) value
  - Problem specific and may need to be tuned

Example

- Traveling Salesman Problem (TSP)
  - Given 6 cities and the traveling cost between any two cities
  - A salesman need to start from city 1 and travel all other cities then back to city 1
  - Minimize the total traveling cost

Example

- Solution representation
  - An integer list, i.e., (1,4,2,3,6,5)
- Search mechanism
  - Swap any two integers (except for the first one)
    - (1,4,2,3,6,5) → (1,4,3,2,6,5)
- Cost function

Example

- Temperature
  - Initial temperature determination
    - Around 80% acceptation rate for “bad move”
    - Determine acceptable (C_{new} – C_{old})
  - Final temperature determination
    - Stop criteria
    - Solution space coverage rate
  - Annealing schedule
    - Constant number (90% for example)
    - Depending on solution space coverage rate

Others

- Global optimal is possible, but near optimal is practical
- Parameter Tuning
  - Aarts, E. and Korst, J. (1989). *Simulated Annealing and Boltzmann Machines*. John Wiley & Sons.
- Not easy for parallel implementation
- Randomly generator

Optimization Techniques

- Mathematical Programming
- Network Analysis
- Branch & Bound
- Genetic Algorithm
- Simulated Annealing
- Tabu Search

Tabu Search

- What
  - Neighborhood search + memory
    - Neighborhood search
    - Memory
      - Record the search history
      - Forbid cycling search

Algorithm

- Choose an initial solution ***x***
- Find a subset of ***N(x)*** the neighbor of ***x*** which are not in the tabu list.
- Find the best one (x') in ***N(x).***
- If F(x') > F(x) then set x=x'.
- Modify the tabu list.
- If a stopping condition is met then stop, else go to the second step.

Effective Tabu Search

- Effective Modeling
  - Neighborhood structure
  - Objective function (fitness or cost)
    - Example Graph coloring problem: Find the minimum number of colors needed such that no two connected nodes share the same color.
- Aspiration criteria
  - The criteria for overruling the tabu constraints and differentiating the preference of among the neighbors

Effective Tabu Search

- Effective Computing
  - “Move” may be easier to be stored and computed than a completed solution
    - move: the process of constructing of x’ from x
  - Computing and storing the fitness difference may be easier than that of the fitness function.

Effective Tabu Search

- **Effective Memory Use**
  - Variable tabu list size
    - For a constant size tabu list

      Too long: deteriorate the search results

      Too short: cannot effectively prevent from cycling
  - Intensification of the search
    - Decrease the tabu list size
  - Diversification of the search
    - Increase the tabu list size
    - Penalize the frequent move or unsatisfied constraints

Example

- A hybrid approach for graph coloring problem
  - R. Dorne and J.K. Hao, *A New Genetic Local Search Algorithm for Graph Coloring*, 1998

Problem

- Given an undirected graph $G=(V,E)$
  - $V=\{v_1,v_2,...,v_n\}$
  - $E=\{e_{ij}\}$
- Determine a partition of V in a minimum number of color classes $C_1,C_2,...,C_k$ such that for each edge e_{ij}, v_i and v_j are not in the same color class.
- NP-hard

General Approach

- Transform an optimization problem into a decision problem
- Genetic Algorithm + Tabu Search
  - Meaningful crossover
  - Using Tabu search for efficient local search

Encoding

- Individual
  - $(C_{i1}, C_{i2}, \ldots, C_{ik})$
- Cost function
  - Number of total conflicting nodes
    - Conflicting node

      having same color with at least one of its adjacent nodes
- Neighborhood (move) definition
  - Changing the color of a conflicting node
- Cost evaluation
  - Special data structures and techniques to improve the efficiency

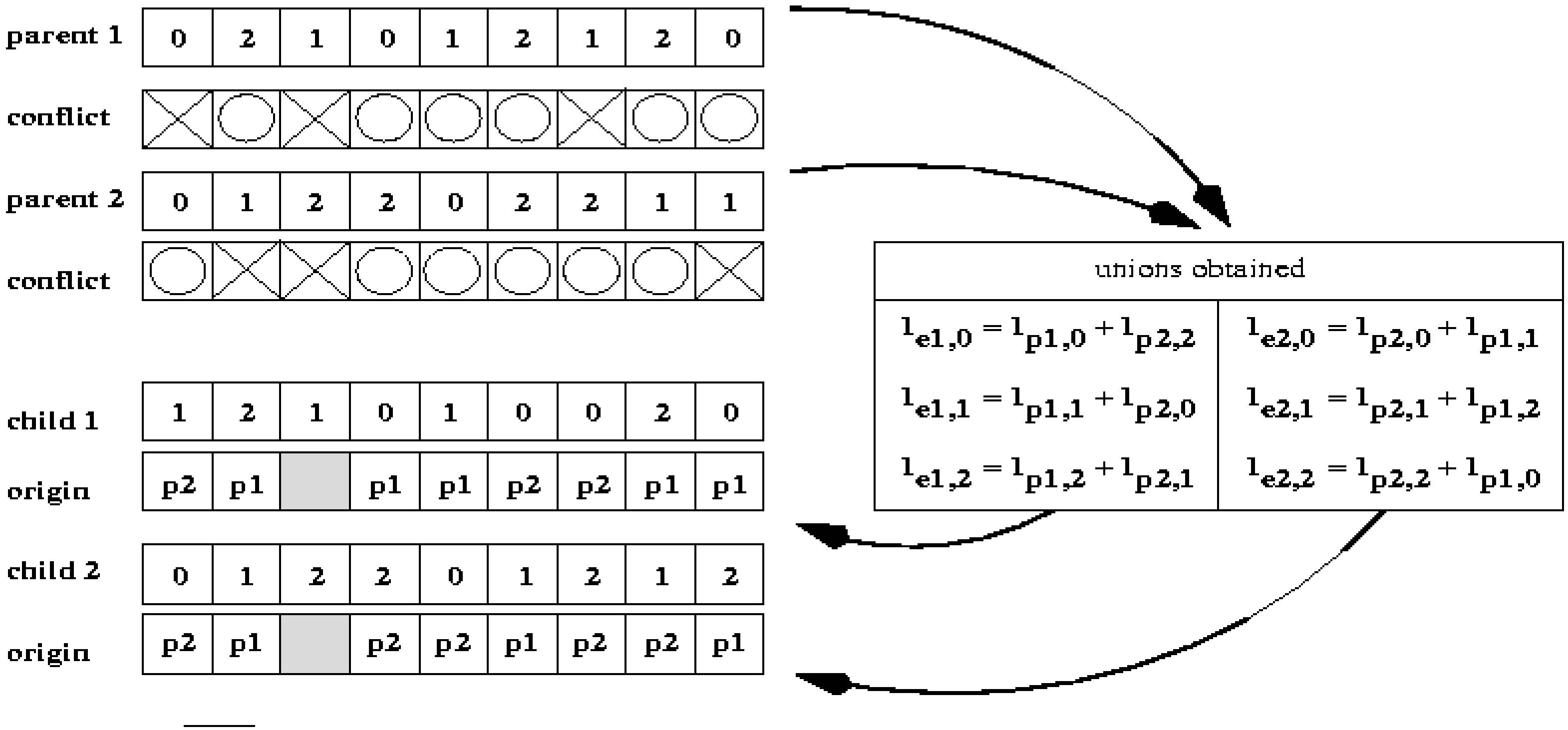
Implementation

- Parent Selection
  - Random
- Reproduction/Survivor
- Crossover Operator
  - Unify independent set (UIS) crossover
    - Independent set

      Conflict-free nodes set with the same color
    - Try to increase the size of the independent set to improve the performance of the solutions

UIS

Unify independent set



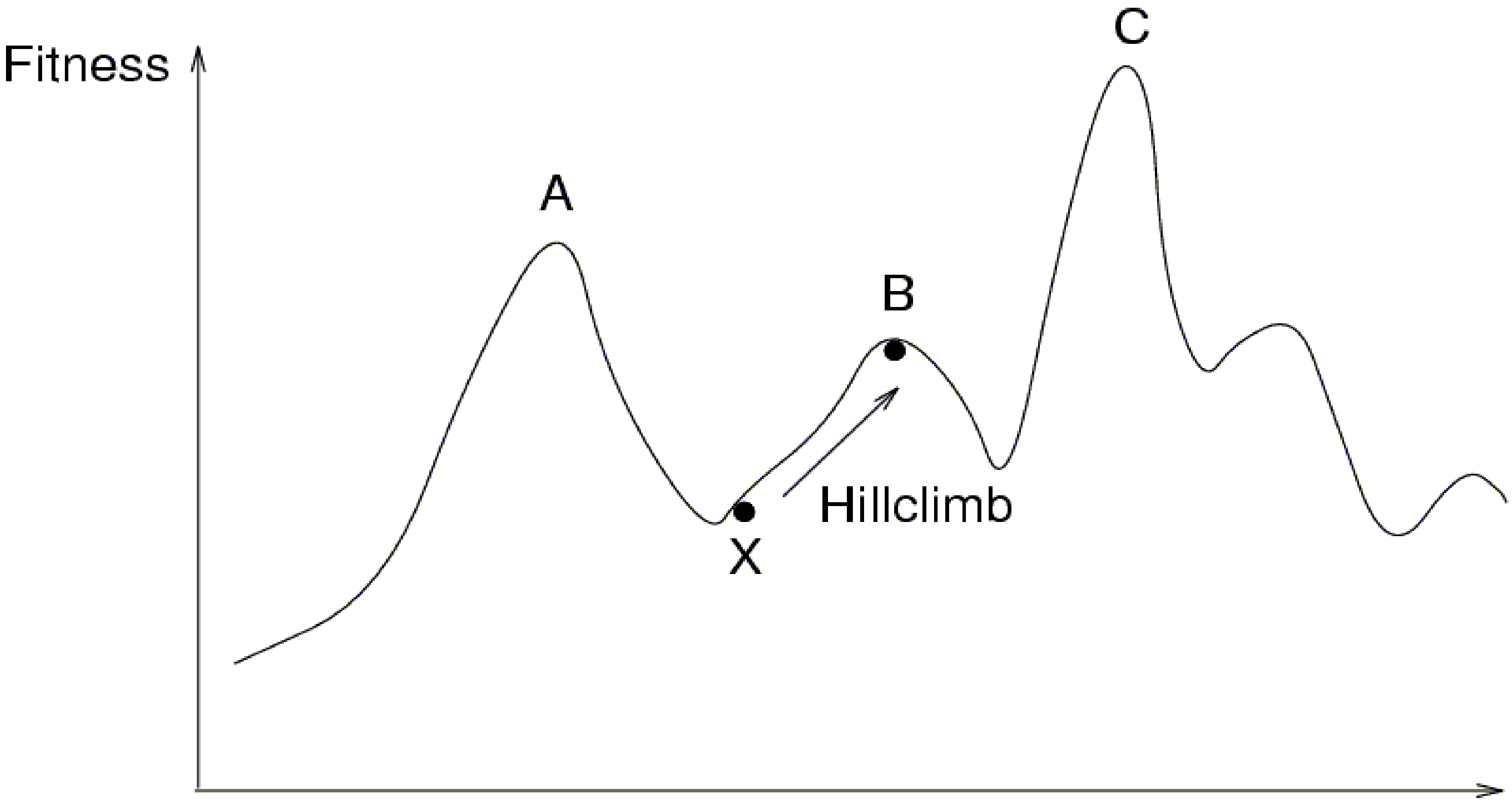
Implementation

- Mutation
  - With Probability P_w, randomly pick neighbor
  - With Probability $1 - P_w$, Tabu search
    - Tabu search
      - Tabu list
        - List of $\{V_i, c_j\}$
      - Tabu tenure (the length of the tabu list)
        - $L = a * N_c + \text{Random}(g)$
        - N_c: Number of conflicted nodes
        - a,g: empirical parameters

Summary

- Neighbor Search
- TS prevent being trapped in the local minimum with tabu list
- TS directs the selection of neighbor
- TS cannot guarantee the optimal result
- Sequential
- Adaptive

Hill climbing



sources

Jaap Hofstede, Beasly, Bull, Martin

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