Algorithms & Complexity
Lecture 6: Randomized Algorithms

November 2, 2020

CentraleSupélec / ESSEC Business School

Dimo Brockhoff

Inria Saclay – Ile-de-France

Corona Update

Taux d'incidence - semaine glissante

ACTIONS

Chiffres-clés 2020-09-11-2020-09-17

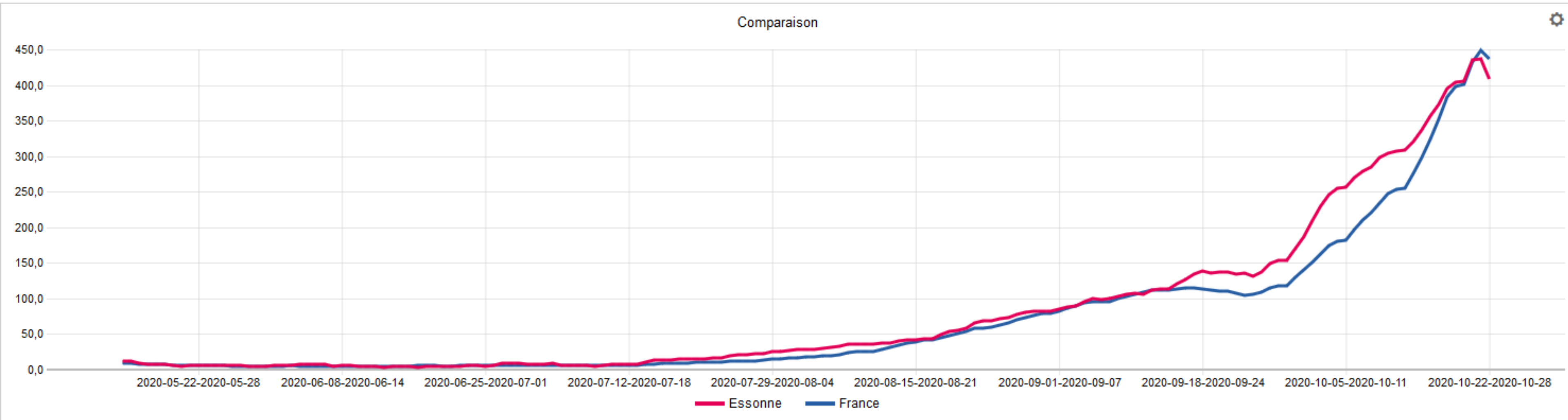
France : **108,1 pour 100 000 hab.**

Essonne : **106,1 pour 100 000 hab.**

Statistique	France
minimum	14,6 (Creuse - 23)
maximum	293,2 (Guadeloupe - 971)
médiane	66,4
observations valides	104 sur 104

Graphiques et comparaisons

Évolution temporelle comparée



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Clarification

Please submit the exercises maximally 3 times with the same student!

…the grade is an individual grade

“In the case of group submissions, please make sure that you submit maximally three times with the same partner!”

[from the exercise sheet(s)]

“Group submissions of 5 students allowed (and highly encouraged!)
But: maximally 3 submissions with the same student pair”

[from the slides]

“Because the grading, however, is individual, I kindly ask that each pair of two students, appears on maximally 3 different solutions.”

[from the webpage]

Clarification

Please submit the exercises maximally 3 times with the same student!

…the grade is an individual grade

Exercise 1 studentA/studentB/studentC, studentD

Exercise 2 studentA/studentB/studentD, studentC

Exercise 3 studentA/studentB/studentC/studentD

Exercise 4 not allowed anymore:

studentA with studentB

allowed one more time:

studentA with studentC

studentA with studentD

studentB with studentC

studentB with studentD

	A	B	C	D
A	-	3	2	2
B	-	-	2	2
C	-	-	-	1
D	-	-	-	-

Discussion Home Exercise

Exercise 1: Greedy Algorithm vs. Dynamic Programming

Correct statements:

a) In a greedy algorithm, we make at each step a decision considering the current situation but don’t look into the future or at the history.

b) It is guaranteed that a dynamic programming approach will generate an optimal solution.

c) A problem should possess the property of non-overlapping subproblems to make None an efficient alternative.

d) A problem should possess the property of overlapping subproblems to make a dynamic programming approach an efficient alternative.

e) A greedy algorithm is more efficient in terms of memory than a dynamic programming approach as it never looks back or revises previous choices.

Exercise 2: Matrix Chain Multiplications

$$A_1 \cdot A_2 \cdots A_n$$

1) Conditions on matrix sizes (A is a_i times b_i matrix):
$$\forall 1 \leq i < n\text{:}\ b_i = a_{i+1}$$
2) Example: 4x3 (matrix) times 3x1 times 1x3 times 3x4
number of calculations:
i) (4x3 times (3x1 times 1x3)) times 3x4 [greedy]
→ $3 \cdot 1 \cdot 3 + 4 \cdot 3 \cdot 3 + 4 \cdot 3 \cdot 4 = 9 + 36 + 48 = 93$
ii) (4x3 times 3x1) times (1x3 times 3x4) [better than greedy]
→ $4 \cdot 3 \cdot 1 + 1 \cdot 3 \cdot 4 + 4 \cdot 1 \cdot 4 = 12 + 12 + 16 = 40$

Definition: $C(i,j)$:= number of calculations to calculate $A_i \cdots A_j$

3) Easy to compute: $C(i,i) = 0$ and $C(i,i+1) = a_i \cdot b_i \cdot b_{i+1}$
4) Sought value (optimum): $C(1,n)$

Discussion Home Exercise

Exercise 2: Matrix Chain Multiplications

5) Assumption: $A_i \cdots A_j$ optimally computed as $(A_i \cdots A_k) \cdot \left(A_{k+1} \cdots A_j\right)$ then: $C(i,j) = C(i,k) + C(k+1,j) + a_i \cdot b_k \cdot b_j$

6) In general:

$$C(i,j) = \begin{cases} 0 & \text{if } i = j \\ a_i \cdot b_i \cdot b_j & \text{if } j = i+1 \\ \min_{i \le k < j} C(i,k) + C(k+1,j) + a_i \cdot b_k \cdot b_j & \text{else} \end{cases}$$

Exercise 2: Matrix Chain Multiplications

7) Matrices: A1 (5-by-2), A2 (2-by-10), A3 (10-by-1), A4 (1-by-10), and A5 (10-by-2)

i/j	1	2	3	4	5
1					
2	-				
3	-	-			
4	-	-	-		
5	-	-	-	-	

Exercise 2: Matrix Chain Multiplications

7) Matrices: A1 (5-by-2), A2 (2-by-10), A3 (10-by-1), A4 (1-by-10), and A5 (10-by-2)

i/j	1	2	3	4	5
1	0	100			
2	-	0	20		
3	-	-	0	100	
4	-	-	-	0	20
5	-	-	-	-	0

Discussion Home Exercise

Exercise 2: Matrix Chain Multiplications

7) Matrices: A1 (5-by-2), A2 (2-by-10), A3 (10-by-1), A4 (1-by-10), and A5 (10-by-2)

i/j	1	2	3	4	5
1	0	100			
2	-	0	20		
3	-	-	0	100	
4	-	-	-	0	20
5	-	-	-	-	0

$$C(1,3) = \min\{0 + 20 + 5 \cdot 2 \cdot 1, 100 + 0 + 5 \cdot 10 \cdot 1\} = \min\{30, 150\}$$

Exercise 2: Matrix Chain Multiplications

7) Matrices: A1 (5-by-2), A2 (2-by-10), A3 (10-by-1), A4 (1-by-10), and A5 (10-by-2)

i/j	1	2	3	4	5
1	0	100	30		
2	-	0	20		
3	-	-	0	100	
4	-	-	-	0	20
5	-	-	-	-	0

$$\mathrm{C}(2,4) = \min\{0 + 100 + 2 \cdot 10 \cdot 10, 20 + 0 + 2 \cdot 1 \cdot 10\} = \min\{300, 40\}$$

Discussion Home Exercise

Exercise 2: Matrix Chain Multiplications

7) Matrices: A1 (5-by-2), A2 (2-by-10), A3 (10-by-1), A4 (1-by-10), and A5 (10-by-2)

i/j	1	2	3	4	5
1	0	100	30		
2	-	0	20	40	
3	-	-	0	100	
4	-	-	-	0	20
5	-	-	-	-	0

$$\mathrm{C}(3,5) = \min\{0+20+10\cdot 1\cdot 2, 100+0+10\cdot 10\cdot 2\} = \min\{40, 300\}$$

Exercise 2: Matrix Chain Multiplications

7) Matrices: A1 (5-by-2), A2 (2-by-10), A3 (10-by-1), A4 (1-by-10), and A5 (10-by-2)

i/j	1	2	3	4	5
1	0	100	30		
2	-	0	20	40	
3	-	-	0	100	40
4	-	-	-	0	20
5	-	-	-	-	0

$$C(1,4) = \min\begin{Bmatrix} 0 + 40 + 5 \cdot 2 \cdot 10 \\ 100 + 100 + 5 \cdot 10 \cdot 10 \\ 30 + 0 + 5 \cdot 1 \cdot 10 \end{Bmatrix} = \min\{140, 700, 80\}$$

Exercise 2: Matrix Chain Multiplications

7) Matrices: A1 (5-by-2), A2 (2-by-10), A3 (10-by-1), A4 (1-by-10), and A5 (10-by-2)

i/j	1	2	3	4	5
1	0	100	30	80	
2	-	0	20	40	
3	-	-	0	100	40
4	-	-	-	0	20
5	-	-	-	-	0

$$C(2,5) = \min \begin{Bmatrix} 0 + 40 + 2 \cdot 10 \cdot 2 \\ 20 + 20 + 2 \cdot 1 \cdot 2 \\ 40 + 0 + 2 \cdot 10 \cdot 2 \end{Bmatrix} = \min\{80, 44{,}80\}$$

Exercise 2: Matrix Chain Multiplications

7) Matrices: A1 (5-by-2), A2 (2-by-10), A3 (10-by-1), A4 (1-by-10), and A5 (10-by-2)

i/j	1	2	3	4	5
1	0	100	30	80	
2	-	0	20	40	44
3	-	-	0	100	40
4	-	-	-	0	20

$$C(1,5) = \min\left\{\begin{matrix} 0 + 44 + 5 \cdot 2 \cdot 2 \\ 100 + 40 + 5 \cdot 10 \cdot 2 \\ 30 + 20 + 5 \cdot 1 \cdot 2 \\ 80 + 0 + 5 \cdot 10 \cdot 2 \end{matrix}\right\} = \min\{64, 240, 60, 180\}$$

Discussion Home Exercise

And the actual solution?

→ need to store where optimum was obtained

-10),

i/j	1	2	3	4	5
1	0	100	30	80	60
2	-	0	20	40	44
3	-	-	0	100	40
4	-	-	-	0	20

$$C(1,5) = \min \begin{Bmatrix} 0 + 44 + 5 \cdot 2 \cdot 2 \\ 100 + 40 + 5 \cdot 10 \cdot 2 \\ 30 + 20 + 5 \cdot 1 \cdot 2 \\ 80 + 0 + 5 \cdot 10 \cdot 2 \end{Bmatrix} = \min\{64, 240, 60, 180\}$$

Discussion Home Exercise

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3	-	-	0	100	40
4	-	-	-	0	20

$$C(1,5) = \min\begin{Bmatrix} 0+44+5\cdot 2\cdot 2 \\ 100+40+5\cdot 10\cdot 2 \\ 30+20+5\cdot 1\cdot 2 \\ 80+0+5\cdot 10\cdot 2 \end{Bmatrix} = \min\{64, 240, 60, 180\}$$

Discussion Home Exercise

And the actual solution?

→ need to store where optimum was obtained

-10),

i/j	1	2	3	4	5
1	0	100	30	80	60
2	-	0			
3	-	-			
4	-	-			

$(A_1 \ldots A_3) \cdot \ (A_4 \cdot A_5)$

then: $(A_1 \cdot (A_2 \cdot A_3)) \cdot \ (A_4 \cdot A_5)$

$$C(1,5) = \min \begin{Bmatrix} 0 + 44 + 5 \cdot 2 \cdot 2 \\ 100 + 40 + 5 \cdot 10 \cdot 2 \\ 30 + 20 + 5 \cdot 1 \cdot 2 \\ 80 + 0 + 5 \cdot 10 \cdot 2 \end{Bmatrix} = \min\{64, 240, 60, 180\}$$

Course Overview

Thu		Topic
Mon, 21.09.2020	PM	Introduction, Combinatorics, O-notation, data structures
Mon, 28.09.2020	AM	Data structures II
Mon, 5.10.2020	AM	Sorting algorithms, recursive algorithms
Mon, 12.10.2020	PM	Greedy algorithms
Mon, 19.10.2020	PM	Dynamic programming
➨ Mon, 2.11.2020	PM	Randomized Algorithms and Blackbox Optimization
Mon, 16.11.2020	AM	Complexity theory I
Mon, 23.11.2020	AM	Complexity theory II
Mon, 14.12.2019	PM	Exam (very likely online)

Randomized Algorithms and Blackbox Optimization

Coping with Difficult Problems

Exact

- brute-force often too slow
- better strategies such as dynamic programming
- still: often exponential runtime

Approximation Algorithms

- guarantee of low run time
- guarantee of high quality solution
- obstacle: often difficult to prove these guarantees

Heuristics

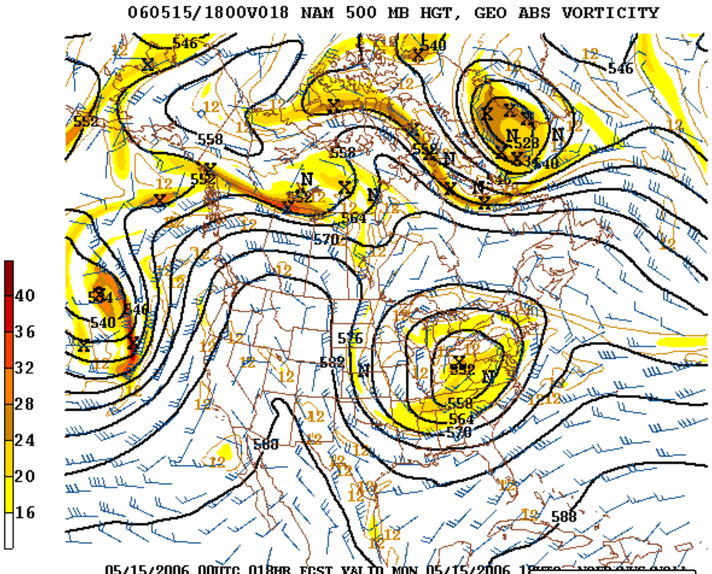
- intuitive algorithms
- guarantee to run in short time
- often no guarantees on solution quality
- designed for practice (become non-heuristic once theoretically analyzed ☺)

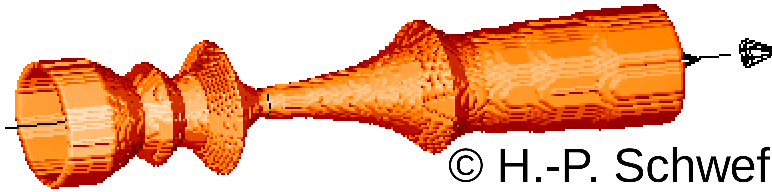
Randomized Algorithms

Randomized Algorithm = Stochastic Algorithm = an algorithm that uses randomness to make decisions

- first proposals in the 1940s (e.g. by N. Metropolis, J. v. Neumann, …) with applications in
  - optimization
  - numerical integration
  - generating draws from a probability distribution
- Monte Carlo algorithm: might not be correct with small probability
- Las Vegas: always correct, but might take long/exponential time

Difficult Optimization Problems are Everywhere





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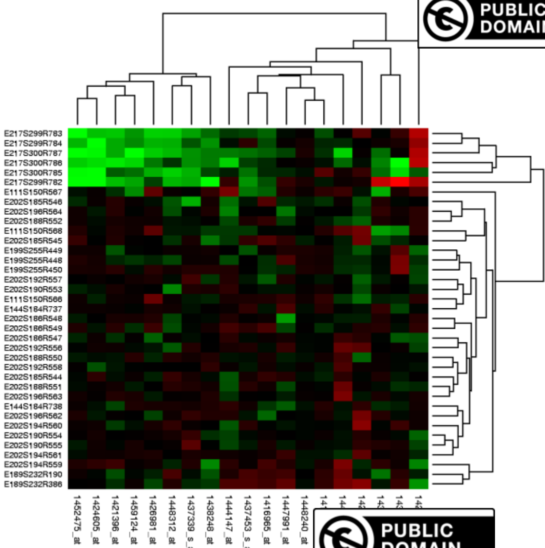
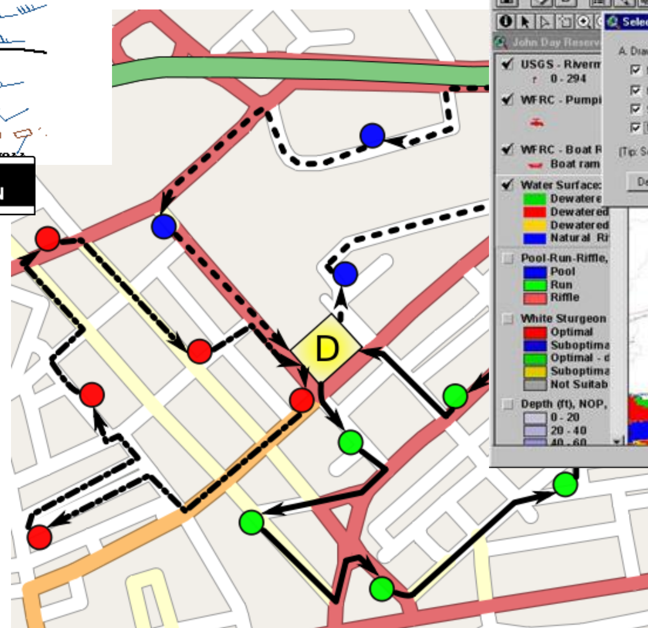
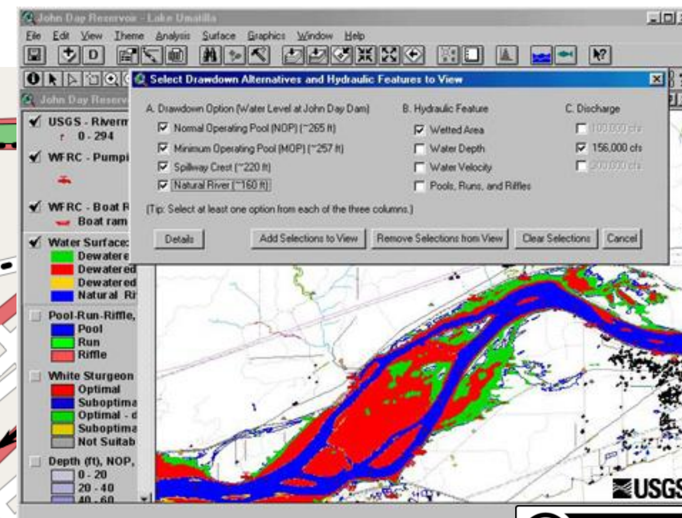




Maly LOLek



What is Optimization?

Typically, we want to

- find solutions x which minimize $f(x)$ in the shortest time possible
  (maximization is reformulated as minimization)

- or find solutions x with as small $f(x)$ in the shortest time possible
  (if finding the exact optimum is not possible)

Black Box Scenario

$x \in \Omega \rightarrow$ **black box** $\rightarrow f(x) \in \mathbb{R}$

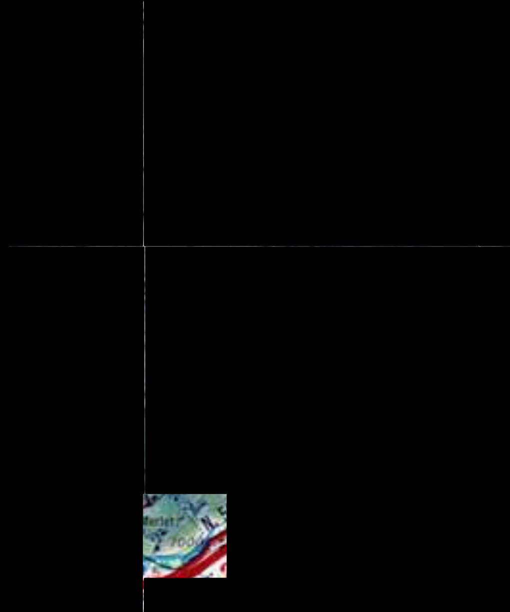
Why are we interested in a black box scenario?

- objective function f often noisy, non-differentiable, or sometimes not even understood or available
- objective function f contains legacy or binary code, is based on numerical simulations or real-life experiments
- most likely, you will see such problems in practice...

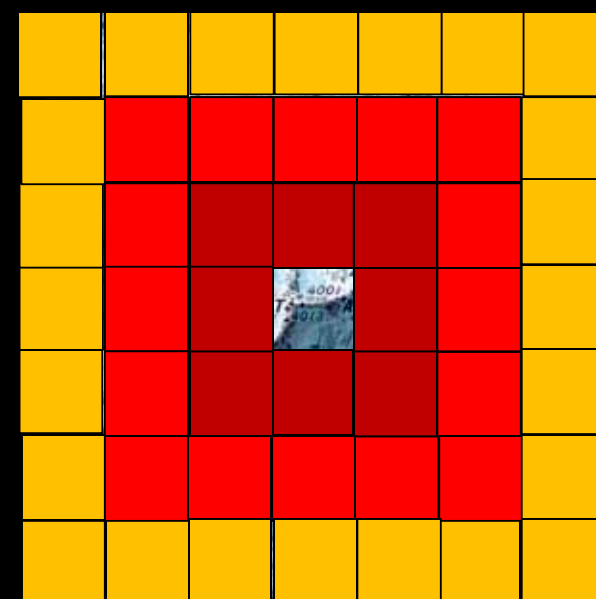
Objective: find x with small $f(x)$ with as few function evaluations as possible

assumption: internal calculations of algo irrelevant

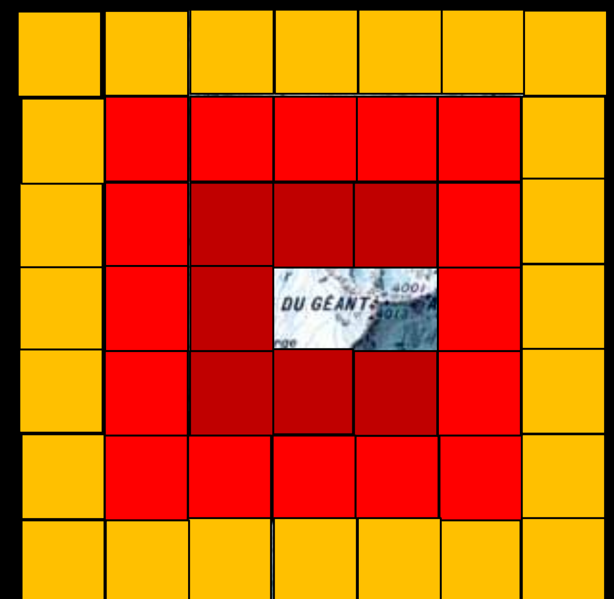
Looks like non-uniform
distributions are better?!



Distribution centered around last (or best) point, with probability decreasing with distance



Distribution centered
around last (or best) point,
with probability decreasing
with distance



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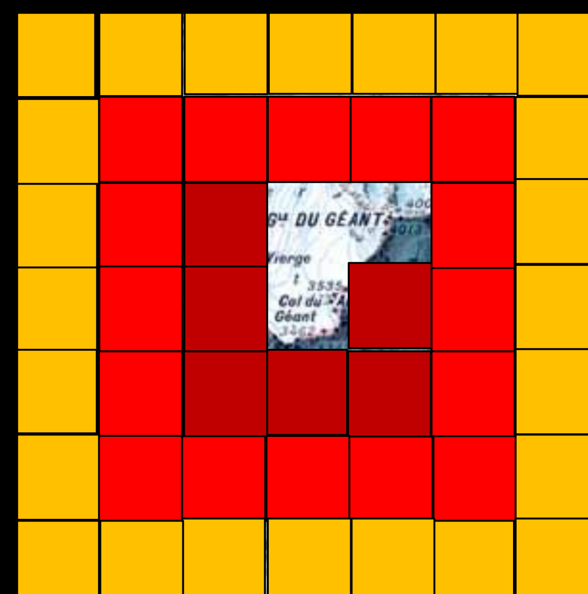

Distribution centered
around last (or best) point,
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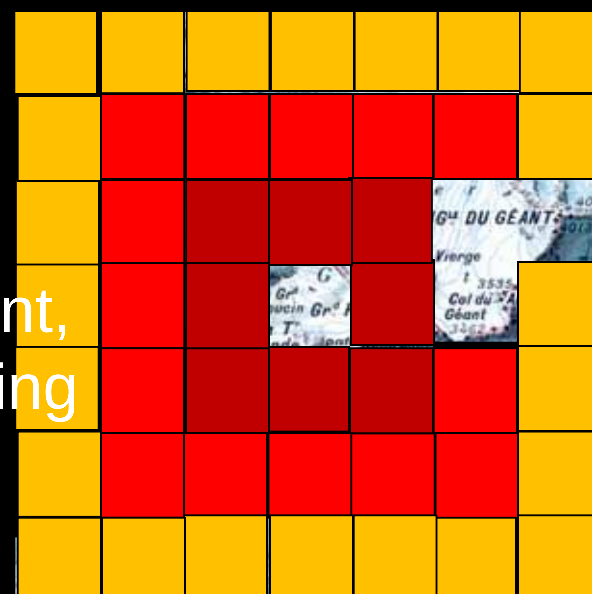


Motivation General Search Heuristics

- often, problem complicated and not much time available to develop a problem-specific algorithm
- general (blackbox) search heuristic: a “meta-algorithm” or “meta-heuristic” which can be applied to a large variety of problems
- search heuristics are a good choice:
  - relatively easy to implement
  - easy to adapt/change/improve
    - e.g. when the problem formulation changes in an early product design phase
    - or when slightly different problems need to be solved over time
- randomized/stochastic algorithms are a good choice because they are robust to noise

Stochastic Search Template

A stochastic blackbox search template to minimize $f: \Omega \to \mathbb{R}$

Initialize distribution parameters θ, set population size $\lambda \in \mathbb{N}$

While happy do:

- Sample distribution $P(\boldsymbol{x}|\theta) \to \boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda \in \Omega$
- Evaluate $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda$ on f
- Update parameters $\theta \leftarrow F_\theta(\theta, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_\lambda, f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_\lambda))$

Deterministic algorithms can be cast in this framework as well:

for example in $\mathbb{R}^n$: gradient descent

or local search in discrete Ω

well-known stochastic example:

Covariance Matrix Adaptation Evolution Strategy (CMA-ES):

sample distributions = multivariate Gaussian distributions

Lecture Outline Randomized Search Heuristics

Here, we touch only algorithms for discrete Ω

❶ Randomized Local Search (RLS)

❷ Evolutionary Algorithms (EAs)

❸ Compact GA: an estimation of distribution algorithm on bitstrings

Neighborhoods

For most (stochastic) search heuristics, we need to define a *neighborhood structure*

- which search points are close to each other?

Example: k-bit flip / Hamming distance k neighborhood

- search space: bitstrings of length n ($\Omega=\{0,1\}^n$)
- two search points are neighbors if their Hamming distance is k
- in other words: x and y are neighbors if we can flip exactly k bits in x to obtain y
- 0001001101 is neighbor of
  0001000101 for k=1
  0101000101 for k=2
  1101000101 for k=3

Neighborhoods II

Example: neighborhoods for permutation problems

- search space: all permutations of length n ($\Omega = S_n$)
- swap neighborhood:
  - swap two entries in the permutation
- equivalence to Hamming distance: swap distance
  - allow to swap k pairs
  - possible to sample in a given distance of k, but algorithm is not trivial
- more neighborhoods for permutations later

Randomized Local Search (RLS)

Idea behind (Randomized) Local Search:

- explore the local neighborhood of the current solution (randomly)

Pure Random Search:

- go to randomly chosen neighbor

First Improvement Local Search:

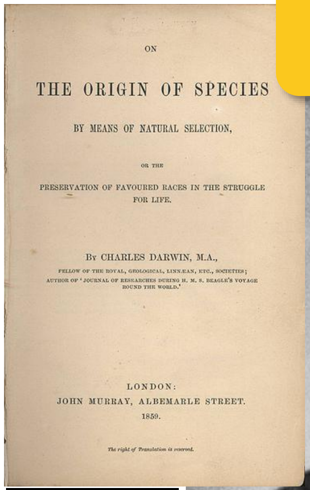
- go to first (randomly) chosen neighbor which is better

Best Improvement strategy:

- always go to the best neighbor
- not random anymore
- computationally expensive if neighborhood large

One class of (bio-inspired) stochastic optimization algorithms: Evolutionary Algorithms (EAs)

1859


ON

THE ORIGIN OF SPECIES

BY MEANS OF NATURAL SELECTION,

OR THE

PRESERVATION OF FAVOURED RACES IN THE STRUGGLE FOR LIFE.

By CHARLES DARWIN, M.A.,

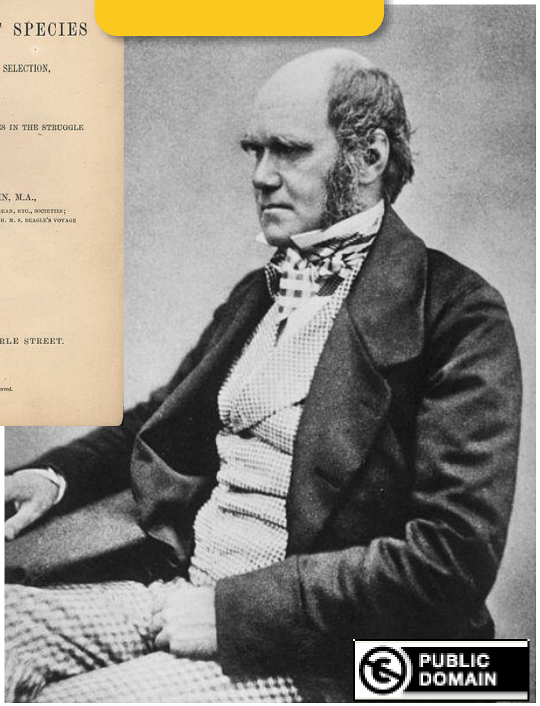
FELLOW OF THE ROYAL, GEOLOGICAL, LINNÆAN, ETC., SOCIETIES; AUTHOR OF 'JOURNAL OF RESEARCHES DURING H. M. S. BEAGLE'S VOYAGE ROUND THE WORLD.'

LONDON:

JOHN MURRAY, ALBEMARLE STREET.

1859.

The right of Translation is reserved.

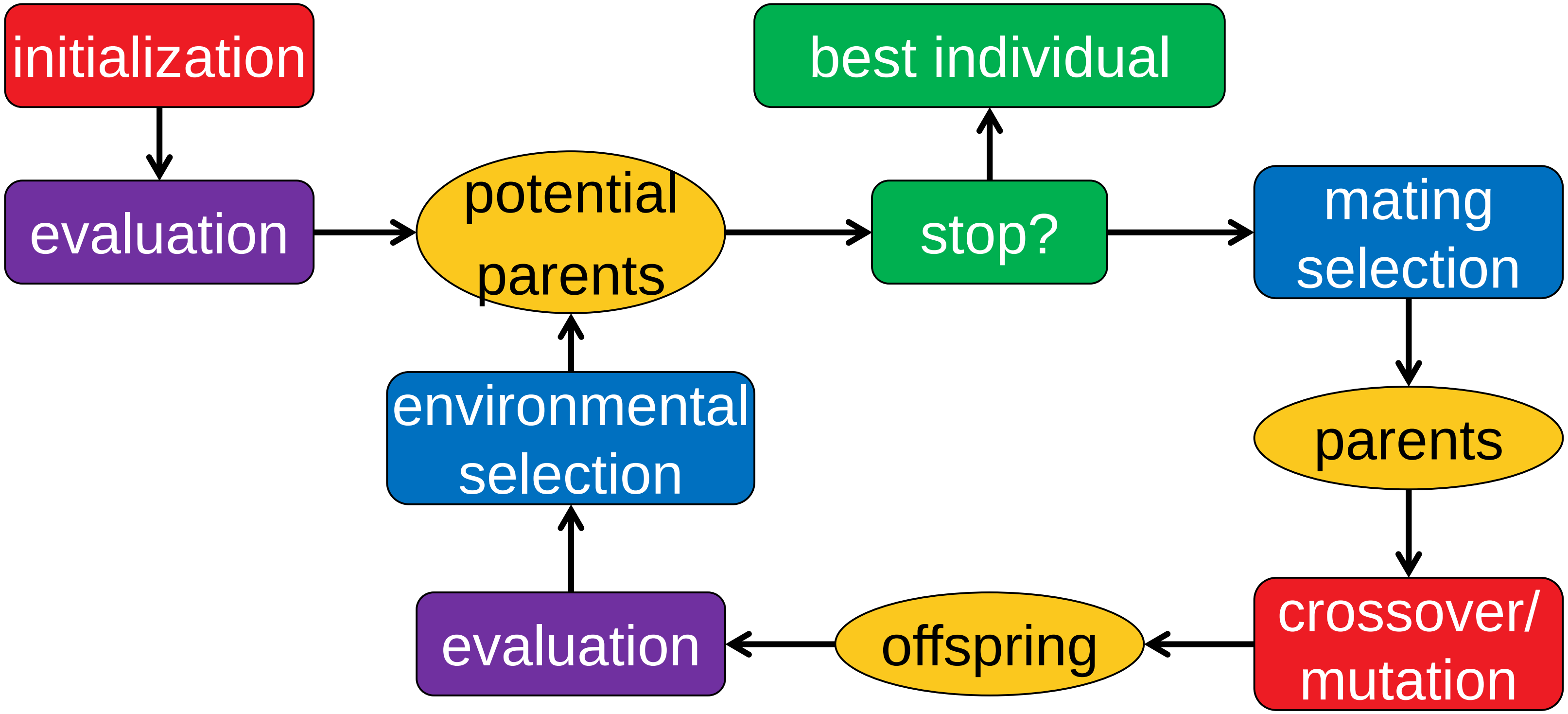


- Class of optimization algorithms originally inspired by the idea of biological evolution
- selection, mutation, recombination

Metaphors

Classical Optimization	Evolutionary Computation
variables or parameters	variables or chromosomes
candidate solution vector of decision variables / design variables / object variables	individual, offspring, parent
set of candidate solutions	population
objective function loss function cost function error function	fitness function
iteration	generation

Generic Framework of an EA



stochastic operators

"Darwinism"

stopping criteria

Important:
representation (search space)

The Historic Roots of EAs

Genetic Algorithms (GA)

J. Holland 1975 and D. Goldberg (USA)

$$\Omega = \{0,1\}^n$$

Evolution Strategies (ES)

I. Rechenberg and H.P. Schwefel, 1965 (Berlin)

$$\Omega = \mathbb{R}^n$$

Evolutionary Programming (EP)

L.J. Fogel 1966 (USA)

Genetic Programming (GP)

J. Koza 1990 (USA)

$$\Omega = \text{space of all programs}$$

nowadays one umbrella term: evolutionary algorithms

Fitness of an individual not always = f(x)

- include constraints
- include diversity
- others
- but needed: always a total order on the solutions

Examples for some EA parts

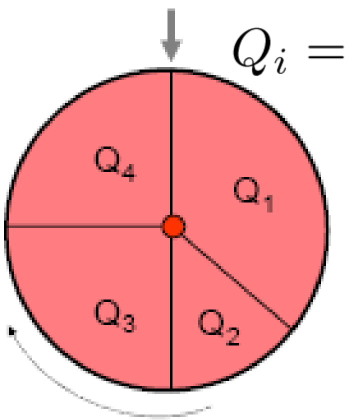
Selection is the major determinant for specifying the trade-off between exploitation and exploration

Selection is either

stochastic or deterministic

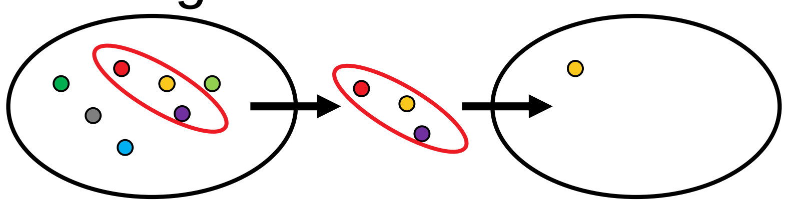
e.g. fitness proportional

$$Q_i = \frac{f(x_i)}{\sum_{j=1}^{\mu} f(x_j)}$$



Disadvantage: depends on scaling of f

e.g. via a tournament



e.g. (μ+λ), (μ,λ)

best μ from offspring *and* parents

best μ from offspring only

Mating selection (selection for variation): usually stochastic

Environmental selection (selection for survival): often deterministic

Variation Operators

Variation aims at generating new individuals on the basis of those individuals selected for mating

Variation = Mutation and Recombination/Crossover

mutation: *mut:* $\Omega \rightarrow \Omega$
recombination: *recomb:* $\Omega^r \rightarrow \Omega^s$ where $r \geq 2$ and $s \geq 1$

- choice always depends on the problem and the chosen representation
- however, there are some operators that are applicable to a wide range of problems and tailored to standard representations such as vectors, permutations, trees, etc.

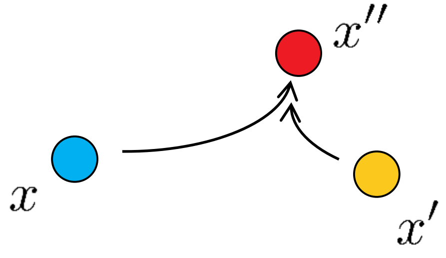
Variation Operators: Guidelines

Two desirable properties for mutation operators:

- every solution can be generation from every other with a probability greater than 0 ("exhaustiveness")
- $d(x, x') < d(x, x'') => Prob(\mathrm{mut}(x) = x') > Prob(\mathrm{mut}(x) = x'')$ ("locality")

Desirable property of recombination operators ("in-between-ness"):

$$x'' = \ \mathrm{recomb}(x, x') \Rightarrow d(x'', x) \leq d(x, x') \wedge d(x'', x') \leq d(x, x')$$



Examples of Mutation Operators on $\{0,1\}^n$

1-bit flip mutation

- flip a randomly chosen bit (from 1 to 0 or vice versa)

k-bit flip mutation

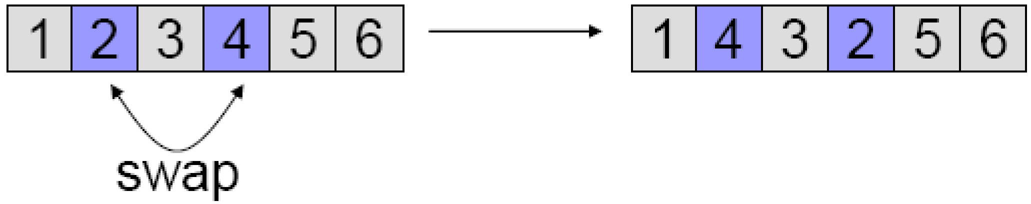
- choose k (different) bits uniformly at random
- flip each of those bits (from 1 to 0 or vice versa)

Standard bitflip mutation

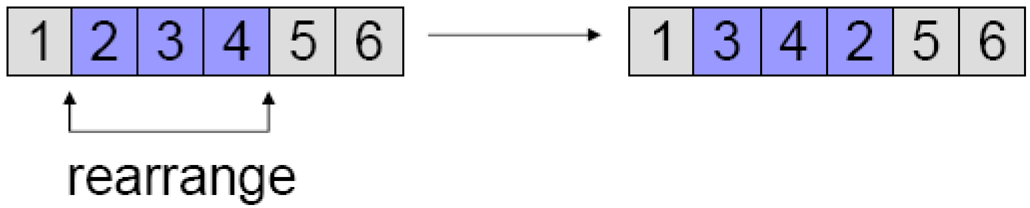
- flip each bit independently with probability 1/n
- expected number of bits changed: 1
- but also: $\lim_{n\to\pm\infty}\left(1-\frac{1}{n}\right)^n = \frac{1}{e} \approx 0.367879$ i.e. no bit flipped with constant probability

Examples of Mutation Operators on Permutations

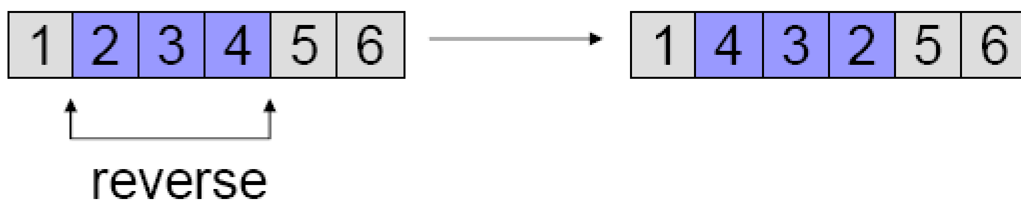
Swap:



Scramble:

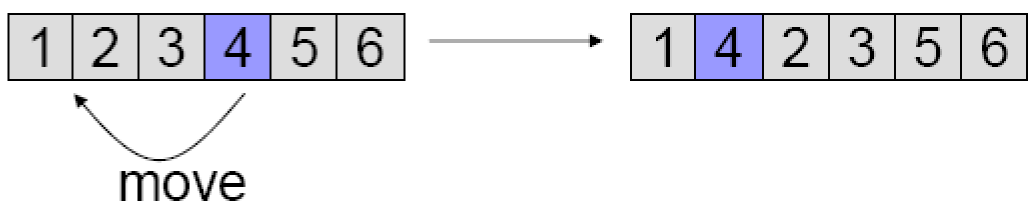


Invert:



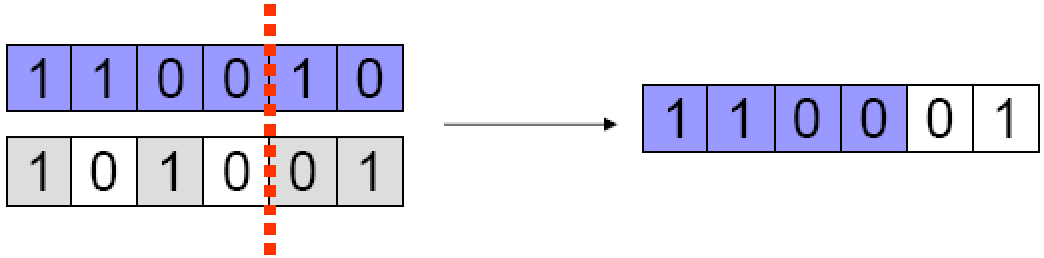
also known as 2-opt

Insert:

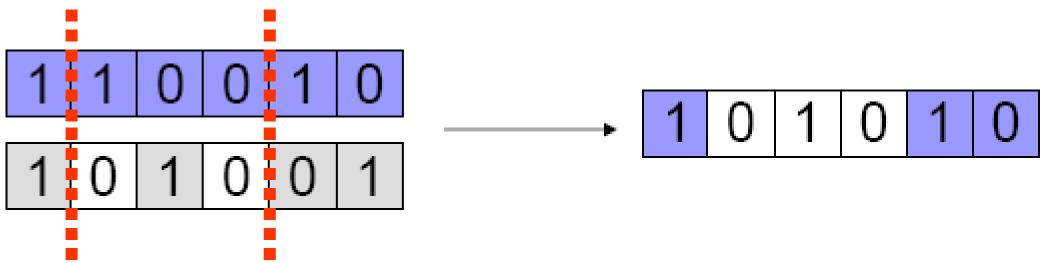


Examples of Recombination Operators on $\{0,1\}^n$

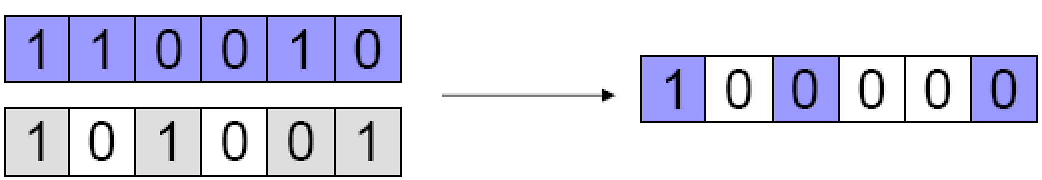
1-point crossover



n-point crossover



uniform crossover



choose each bit independently from one parent or another

A Canonical Genetic Algorithm

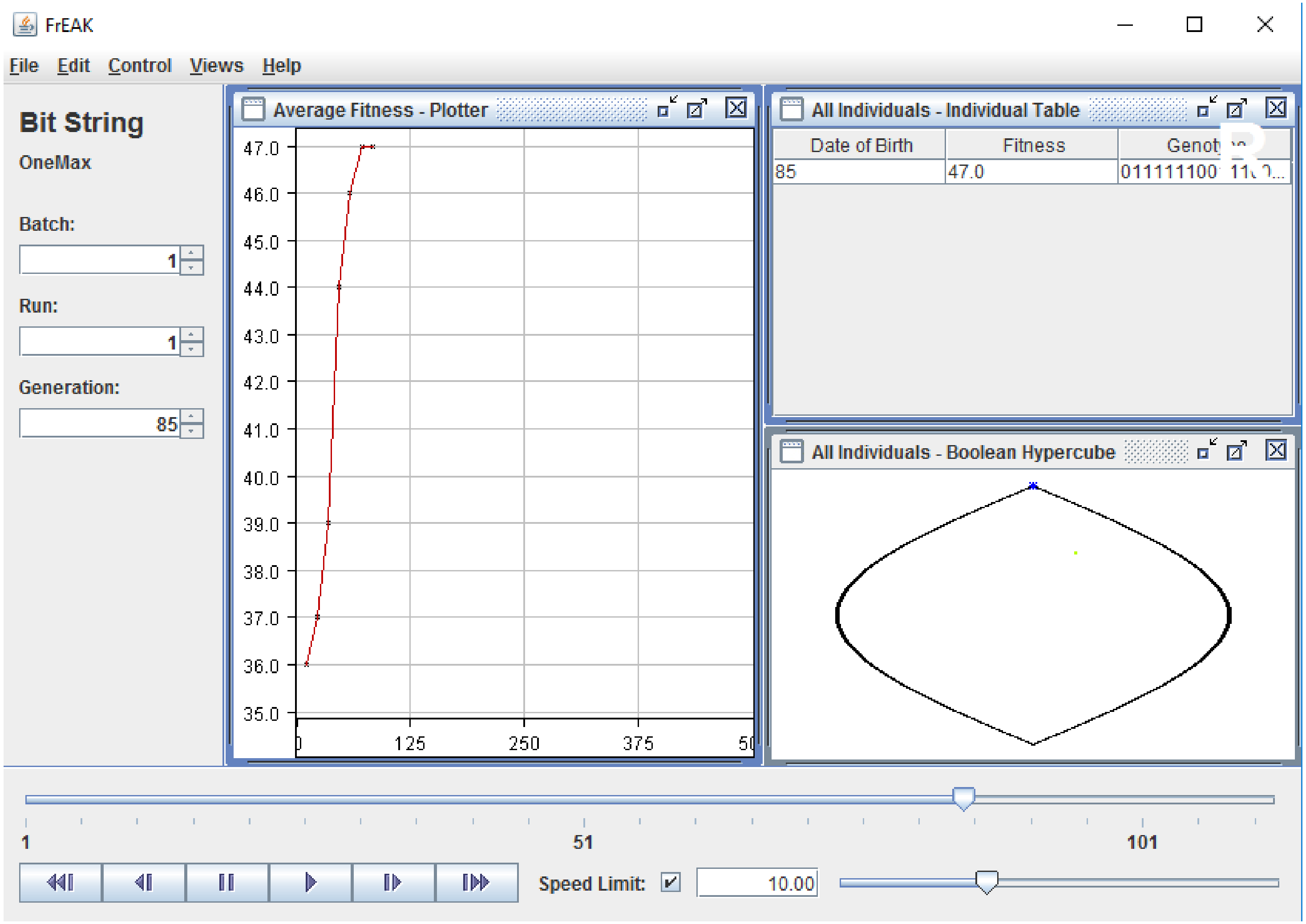
- binary search space, maximization
- uniform initialization
- generational cycle:
  - evaluation of solutions
  - mating selection (e.g. roulette wheel)
  - crossover (e.g. 1-point)
  - environmental selection (e.g. plus-selection)

You may ask: how does this fit
into the stochastic search template?
it does: population contained in state θ,
but update function difficult to write down

FrEAK

If you want to play around a bit with these algorithms:

- https://sourceforge.net/projects/freak427/



Estimation of Distribution Algorithms

- Estimation of Distribution Algorithms (EDAs) fit more obviously into the search template
- here, example of the compact Genetic Algorithm (cGA)
  - search space: $\Omega = \{0,1\}^n$
  - probability distribution: Bernoulli
    - store for each bit a probability p_i to sample a 1
    - sample bit i with probability p_i to 1 and with $(1 - p_i)$ to 0

The Compact GA

Parameters: number of variables n, learning rate K (typically $= n$)

Init:

$p = \left(\frac{1}{2}, \frac{1}{2}, \dots, \frac{1}{2}\right) \in [0,1]^n$ # probabilities to sample new solutions

While happy:

create $S = (s_1, \dots, s_n)$ by sampling each s_i with probability p_i

create $S' = (s'_1, \dots, s'_n)$ by sampling each s'_i with probability p_i

evaluate S and S' on f

if $f(S) > f(S')$: # make sure that S is the better solution

$S, S' \leftarrow S', S$

update p parameter:

for $i \in \{1, \dots, n\}$:

$p_i \leftarrow \min\{\max\{p_i + (s_i - s'_i)/K, 1/n\}, 1 - 1/n\}$

return S

Conclusions

- EAs are generic algorithms (randomized search heuristics, meta-heuristics, ...) for black box optimization

  no or almost no assumptions on the objective function

- They are typically less efficient than problem-specific (exact) algorithms in discrete domain (in terms of #funevals)

  but competitive in the continuous case

- Allow for an easy and rapid implementation and therefore to find good solutions fast

  easy (recommended!) to incorporate problem-specific knowledge to improve the algorithm

Conclusions

I hope it became clear...

...that heuristics is what we typically can afford in practice (no guarantees and no proofs)

...what are the main ideas behind evolutionary algorithms

...and that evolutionary algorithms and genetic algorithms are no synonyms