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Witt, Carsten

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Theory of Randomized Search Heuristics in Combinatorial Optimization

Carsten Witt

DTU Informatics
Technical University of Denmark
www.imm.dtu.dk/~cawi

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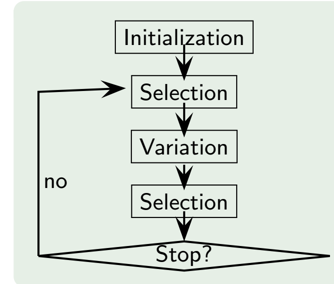
Evolutionary Algorithms and Other Search Heuristics

Most famous search heuristic: Evolutionary Algorithms (EAs)

- a bio-inspired heuristic
- paradigm: evolution in nature, "survival of the fittest"



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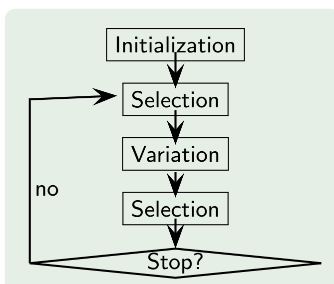

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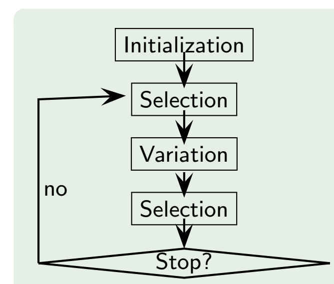
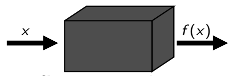


- Goal: optimization
- Here: discrete search spaces, combinatorial optimization, in particular pseudo-boolean functions

Optimize $f\colon \{0,1\}^n \to \mathbb{R}$

Why Do We Consider Randomized Search Heuristics?

- Not enough resources (time, money, knowledge) for a tailored algorithm
- Black Box Scenario 

  rules out problem-specific algorithms
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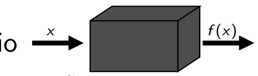
- Black Box Scenario 

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- They are surprisingly successful.

Point of view

Do not only consider RSHs empirically. We need a solid theory to understand how (and when) they work.

What RSHs Do We Consider?

Theoretically considered RSHs

- (1+1) EA
- (1+λ) EA (offspring population)
- (μ+1) EA (parent population)
- (μ+1) GA (parent population and crossover)
- GIGA (crossover)
- SEMO, DEMO, FEMO, ... (multi-objective)
- Randomized Local Search (RLS)
- Metropolis Algorithm/Simulated Annealing (MA/SA)
- Ant Colony Optimization (ACO)
- Particle Swarm Optimization (PSO)
- ...

First of all: define the simple ones

The Most Basic RSHs

(1+1) EA, RLS, MA and SA for maximization problems

(1+1) EA

1. Choose $x_0 \in \{0,1\}^n$ uniformly at random.
2. For $t := 0, \dots, \infty$
   1. Create y by flipping each bit of x_t indep. with probab. $1/n$.
   2. If $f(y) \geq f(x_t)$ set $x_{t+1} := y$ else $x_{t+1} := x_t$.

The Most Basic RSHs

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RLS

1. Choose $x_0 \in \{0,1\}^n$ uniformly at random.
2. For $t := 0, \dots, \infty$
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The Most Basic RSHs

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MA

1. Choose $x_0 \in \{0,1\}^n$ uniformly at random.
2. For $t := 0, \dots, \infty$
   1. Create y by flipping one bit of x_t uniformly.
   2. If $f(y) \geq f(x_t)$ set $x_{t+1} := y$
      else $x_{t+1} := y$ with probability $e^{(f(x_t)-f(y))/T}$ anyway
      and $x_{t+1} := x_t$ otherwise.

T is fixed over all iterations.

The Most Basic RSHs

(1+1) EA, RLS, MA and SA for maximization problems

SA

1. Choose $x_0 \in \{0,1\}^n$ uniformly at random.
2. For $t := 0, \dots, \infty$
   1. Create y by flipping one bit of x_t uniformly.
   2. If $f(y) \geq f(x_t)$ set $x_{t+1} := y$
      else $x_{t+1} := y$ with probability $e^{(f(x_t)-f(y))/T_t}$ anyway
      and $x_{t+1} := x_t$ otherwise.

T_t is dependent on t, typically decreasing

What Kind of Theory Are We Interested in?

- Not studied here: convergence, local progress, models of EAs (e. g., infinite populations), ...
- Treat RSHs as randomized algorithm!
- Analyze their "runtime" (computational complexity) on selected problems

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Definition

Let RSH A optimize f. Each f-evaluation is counted as a time step. The *runtime* $T_{A,f}$ of A is the random first point of time such that A has sampled an optimal search point.

- Often considered: expected runtime, distribution of $T_{A,f}$
- Asymptotical results w. r. t. n

How Do We Obtain Results?

We use (rarely in their pure form):

- Coupon Collector's Theorem
- Principle of Deferred Decisions
- Concentration inequalities:
  Markov, Chebyshev, Chernoff, Hoeffding, ... bounds
- Markov chain theory: waiting times, first hitting times
- Rapidly Mixing Markov Chains
- Random Walks: Gambler's Ruin, drift analysis (Wald's equation), martingale theory, electrical networks
- Random graphs (esp. random trees)
- Identifying typical events and failure events
- Potential functions and amortized analysis
- ...

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Adapt tools from the analysis of randomized algorithms; understanding the stochastic process is often the hardest task.

Early Results

Analysis of RSHs already in the 1980s:

- Sasaki/Hajek (1988): SA and Maximum Matchings
- Sorkin (1991): SA vs. MA
- Jerrum (1992): SA and Cliques
- Jerrum/Sorkin (1993, 1998): SA/MA for Graph Bisection
- ...

These were high-quality results, however, limited to SA/MA (nothing about EAs) and hard to generalize.

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Since the early 1990s

Systematic approach for the analysis of RSHs, building up a completely new research area

This Tutorial

1. The origins: example functions and toy problems
   - A simple toy problem: OneMax for (1+1) EA
2. Combinatorial optimization problems
   - (1+1) EA and minimum spanning trees
   - (1+1) EA and Eulerian cycles
   - (1+1) EA and maximum matchings
   - (1+1) EA and the partition problem
   - SA beats MA in combinatorial optimization
3. End

How the Systematic Research Began — Toy Problems

Simple example functions (test functions)

- $\text{OneMax}(x_1, \dots, x_n) = x_1 + \dots + x_n$
- $\text{LeadingOnes}(x_1, \dots, x_n) = \sum_{i=1}^{n} \prod_{j=1}^{i} x_j$
- $\text{BinVal}(x_1, \dots, x_n) = \sum_{i=1}^{n} 2^{n-i} x_i$
- polynomials of fixed degree

Goal: derive first runtime bounds and methods

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Artificially designed functions

- with sometimes really horrible definitions
- but for the first time these allow rigorous statements

Goal: prove benefits and harm of RSH components, e. g., crossover, mutation strength, population size ...

Agenda

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Example: OneMax

Theorem (e. g., Droste/Jansen/Wegener, 1998)
The expected runtime of the RLS, (1+1) EA, (μ+1) EA, (1+λ) EA on OneMax *is* $\Omega(n \log n)$.

Proof by modifications of Coupon Collector's Theorem.

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Proof by modifications of Coupon Collector's Theorem.

Theorem (e. g., Mühlenbein, 1992)
The expected runtime of RLS and the (1+1) EA on OneMax *is* $O(n \log n)$.

Holds also for population-based (μ+1) EA and for (1+λ) EA with small populations.

Proof of the $O(n \log n)$ bound

- *Fitness levels:* $L_i := \{x \in \{0,1\}^n \mid \textsc{OneMax}(x) = i\}$

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Proof of the $O(n \log n)$ bound

- *Fitness levels:* $L_i := \{x \in \{0,1\}^n \mid \text{OneMax}(x) = i\}$
- (1+1) EA never decreases its current fitness level.
- From i to some higher-level set with prob. at least

$$\underbrace{\binom{n-i}{1}}_{\text{choose a 0-bit}} \cdot \underbrace{\binom{1}{n}}_{\text{flip this bit}} \cdot \underbrace{\left(1-\frac{1}{n}\right)^{n-1}}_{\text{keep the other bits}} \geq \frac{n-i}{en}$$

- Expected time to reach a higher-level set is at most $\frac{en}{n-i}$.
- Expected runtime is at most

$$\sum_{i=0}^{n-1} \frac{en}{n-i} = O(n \log n). \qquad \square$$

Later Results Using Toy Problems

- Find the theoretically optimal mutation strength ($1/n$ for OneMax!).
- Bound the optimization time for linear functions ($O(n \log n)$).
- optimal population size (often 1!)
- crossover vs. no crossover → Real Royal Road Functions
- multistarts vs. populations
- frequent restarts vs. long runs
- dynamic schedules
- ...

RSHs for Combinatorial Optimization

- Analysis of runtime and approximation quality on well-known combinatorial optimization problems, e. g.,
  - sorting problems (is this an optimization problem?),
  - covering problems,
  - cutting problems,
  - subsequence problems,
  - traveling salesperson problem,
  - Eulerian cycles,
  - minimum spanning trees,
  - maximum matchings,
  - scheduling problems,
  - shortest paths,
  - ...

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  - ...
- What we do not hope: to be better than the best problem-specific algorithms
- In the following no fine-tuning of the results
- More details in the books (last slide)

Agenda

Minimum Spanning Trees

Problem

Given: Undirected connected graph $G = (V, E)$ with n vertices and m edges with positive integer weights.
Find: Edge set $E' \subseteq E$ with minimal weight connecting all vertices.

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Fitness function

Decrease number of connected components, find minimum spanning tree:

$$f(s) := (c(s), w(s)).$$

Minimization of f with respect to the lexicographic order.

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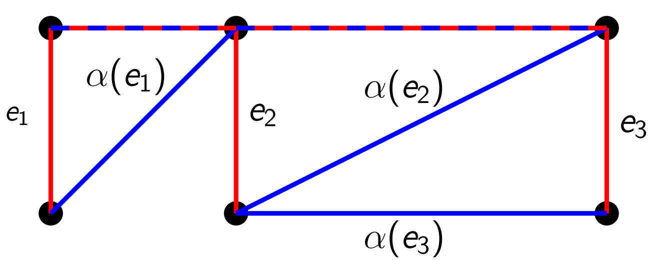
Connected graph

- Connected graph in expected time $O(m \log n)$ (fitness level arguments)

Combinatorial Argument to Approach MSTs

From arbitrary spanning tree T to MST T^* (Mayr/Plaxton, 1992):



- $k := |E(T^*) \setminus E(T)|$
- Bijection $\alpha : E(T^*) \setminus E(T) \to E(T) \setminus E(T^*)$
- $\alpha(e_i)$ on the cycle of $E(T) \cup \{e_i\}$
- $w(e_i) \leq w(\alpha(e_i))$

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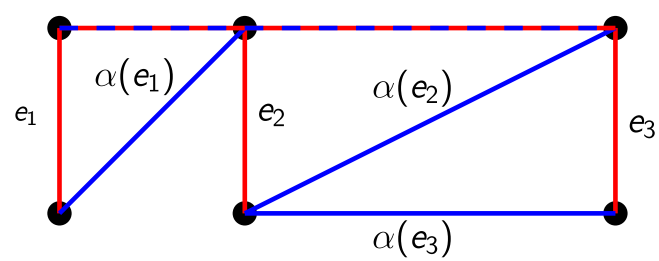

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- $w(e_i) \leq w(\alpha(e_i))$

$\Longrightarrow$ k accepted 2-bit flips that turn T into T^*

Upper Bound

Theorem (Neumann/Wegener, 2007)

The expected time until (1+1) EA constructs a minimum spanning tree is bounded by $O(m^2(\log n + \log w_{\max}))$.

Sketch of proof:

- $w(s)$ weight current solution s; assume to be tree
- w_{opt} weight minimum spanning tree T^*

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Sketch of proof:

- $w(s)$ weight current solution s; assume to be tree
- w_{opt} weight minimum spanning tree T^*
- set of n operations to reach T^*
  - k 2-bit flips defined by bijection
  - $n - k$ non accepted 2-bit flips
- $\Longrightarrow$ average weight decrease $(w(s) - w_{opt})/n$

Upper Bound

Concentrate on 2-bit flips:

- Expected weight decrease by a factor $1 - 1/n$ (or better)
- Probability $\Theta(n/m^2)$ for a good 2-bit flip
- Expected time until r 2-steps $O(rm^2/n)$

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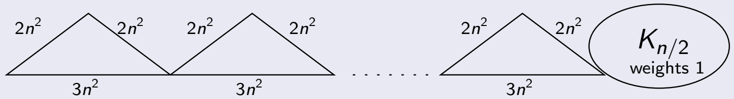
Method expected multiplicative distance decrease:

- Have to bridge distance at most $D := w(s) - w_{\text{opt}} \leq m \cdot w_{\max}$.
- Distance after N steps: $\leq (1 - 1/n)^N \cdot D$
- Find N such that $(1 - 1/n)^N \leq 1/(2D)$
  $\Rightarrow$ choose $N := \lceil n \cdot (\ln D + 1) \rceil$
- In expectation $2N = O(n(\log n + \log w_{max}))$ 2-steps enough
- Expected time: $O(Nm^2/n) = O(m^2(\log n + \log w_{\max}))$

Further Results

Lower Bound $\Omega(n^4 \log n)$



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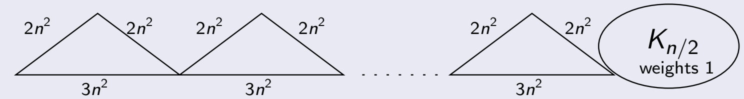

Related Results

- Experimental investigations (Briest et al., 2004)
- Biased mutation operators (Raidl/Koller/Julstrom, 2006)
- $O(mn^2)$ for a multi-objective approach (Neumann/Wegener, 2006)
- Approximations for multi-objective minimum spanning trees (Neumann, 2007)
- SA/MA and minimum spanning trees (Later!)

Agenda

Eulerian Cycle Problem

Given: undirected connected Eulerian (degree of each vertex is even) graph $G = (V, E)$ with n vertices and m edges

Find: a cycle (permutation of the edges) such that each edge is used exactly once.

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Eulerian Cycle (Hierholzer)

Idea: "glue" small cycles together

1. Find a cycle C in G.
2. Delete the edges of C from G.
3. If G is not empty go to step 1; starting from a vertex on C.
4. Construct the Eulerian cycle by running through the cycles produced in Step 1 in the order of construction.

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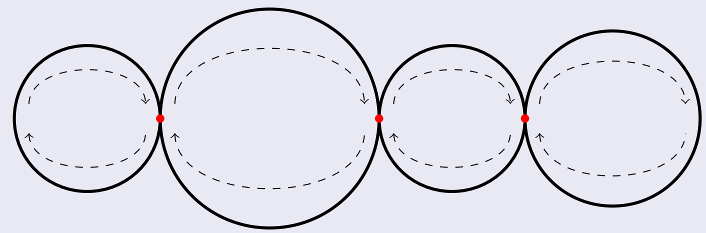

Fitness Function

Representation: permutation of edges

Fitness function

Consider the edges of the permutation after another and build up a path p of length l.

$$\text{path}(\pi) := \textit{length of the path } p \textit{ implied by } \pi$$

Example: $\pi = (\{2,3\}, \{1,2\}, \{1,5\}, \{3,4\}, \{4,5\}) \Longrightarrow |p| = 3$

The (1+1) EA for the Euler Cycle Problem

(1+1) EA

1. Choose $\pi \in S_m$ uniform at random.
2. Choose s from a Poisson distribution with parameter 1. Perform sequentially $s + 1$ jump operations to produce π' from π.

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   Example: jump(2,4) applied to
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   Example: jump(2,4) applied to
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   ({2,3},{3,4},{1,5},{1,2},{4,5})
3. Replace π by π' if path(π') $\geq$ path(π).
4. Repeat Steps 2 and 3 forever.

Upper Bound, (1+1) EA

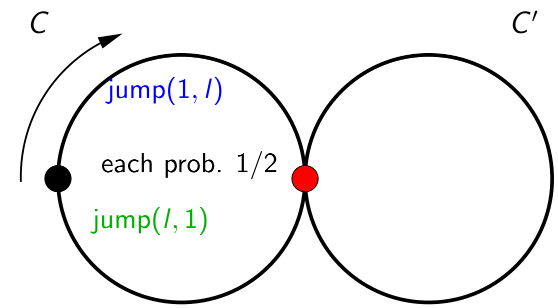
Theorem (Neumann, 2007)

The expected time until (1+1) EA working on the fitness function path constructs an Eulerian cycle is bounded by $O(m^5)$.

Proof idea:

- p is not a cycle:
  1 improving jump $\Rightarrow$ expected time for improvement $O(m^2)$
- p is a cycle (with less than m edges):
  Show: expected time for an improvement $O(m^4)$
- $O(m)$ improvements $\Rightarrow$ theorem

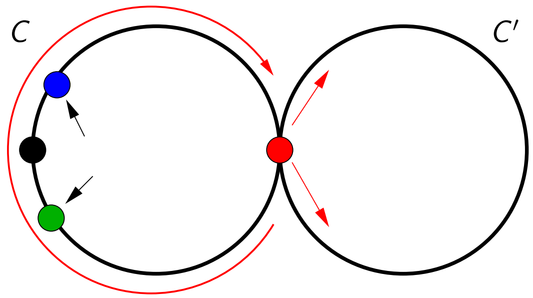
Proof Idea: How to Analyze Improvements



Typical run:

- k-step (accepted mutation with k-jumps that change p)
- Only 1-steps: $O(m^4)$ steps for an improvement
- No k-step, $k \geq 4$, in $O(m^4)$ steps with prob. $1 - o(1)$
- $O(1)$ 2- or 3-steps in $O(m^4)$ steps with prob. $1 - o(1)$

Proof Idea: How to Shift a Cycle



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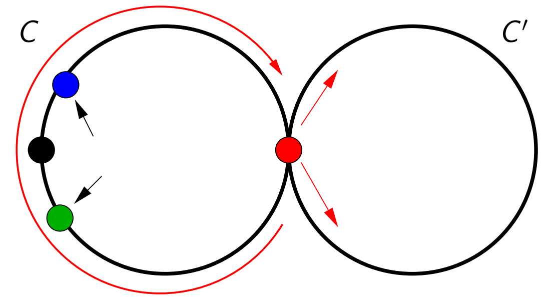

- Time $O(m^2)$ to move black vertex
- Black vertex performs random walk
- Length of cycle at most m
- Fair random walk
  $\rightarrow O(m^2)$ movements are enough to reach red vertex
- Expected time for an improvement $O(m^4)$

Further Results

- Lower bound $\Omega(m^4)$

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- Restricted jumps (always jump to position 1)
  - No random walk, but directed walk
  - Upper bound $O(m^3)$ (Doerr/Hebbinghaus/Neumann, 2007)

Further Results

- Lower bound $\Omega(m^4)$
- Restricted jumps (always jump to position 1)
  - No random walk, but directed walk
  - Upper bound $O(m^3)$ (Doerr/Hebbinghaus/Neumann, 2007)
- Use of more sophisticated representations and mutation operators:
  - $O(m^2 \log m)$ (Doerr/Klein/Storch, 2007)
  - $O(m \log m)$ (Doerr/Johannsen, 2007)

Agenda

(1+1) EA for the Maximum Matching Problem
The Behavior on Paths

A matching in a graph is a subset of pairwise disjoint edges.

Path: $n+1$ nodes, n edges: bit string from $\{0,1\}^n$ selects edges

Fitness function: size of matching/negative for non-matchings

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A matching in a graph is a subset of pairwise disjoint edges.

Path: $n+1$ nodes, n edges: bit string from $\{0,1\}^n$ selects edges

Fitness function: size of matching/negative for non-matchings

Theorem (Giel/Wegener, 2003)

The expected time until the (1+1) EA finds a maximum matching on a path of n edges is $O(n^4)$.

(1+1) EA for the Maximum Matching Problem
The Behavior on Paths (2)

Proof idea:

- Consider a second-best matching.
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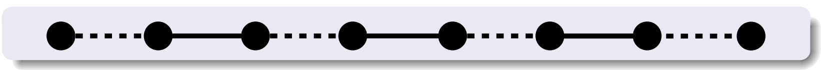

(1+1) EA for the Maximum Matching Problem
The Behavior on Paths (2)

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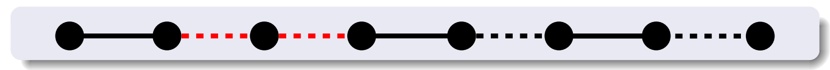

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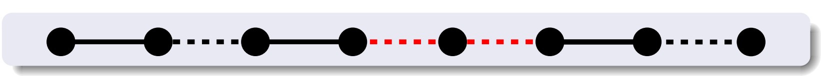

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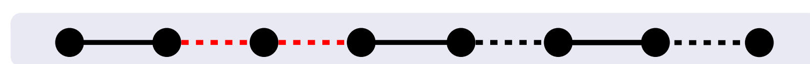

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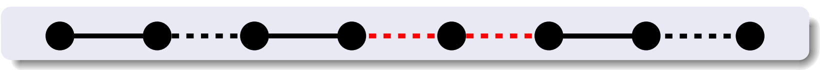

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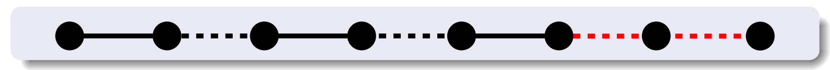

32/48
Carsten Witt Theory of RSH in Combinatorial Optimization

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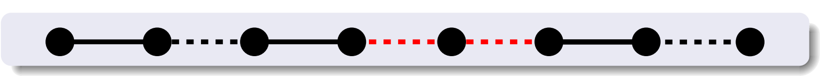

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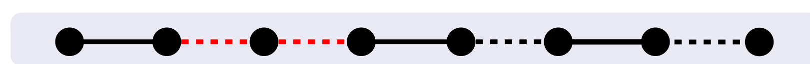

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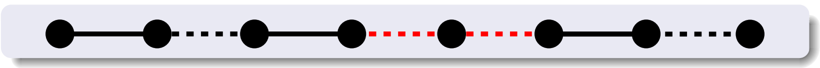

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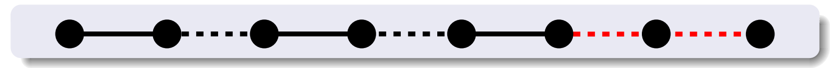

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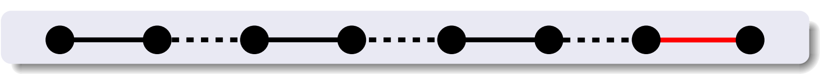

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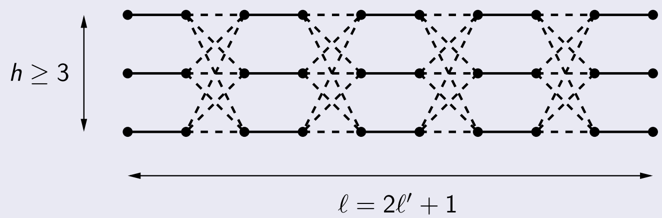
- Length changes according to a fair random walk
  $\rightarrow$ Expected runtime $O(n^2) \cdot O(n^2) = O(n^4)$.

Worst-case graph $G_{h,\ell}$ (Sasaki/Hajek, 1988)



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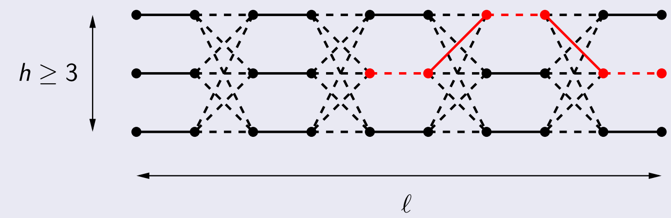
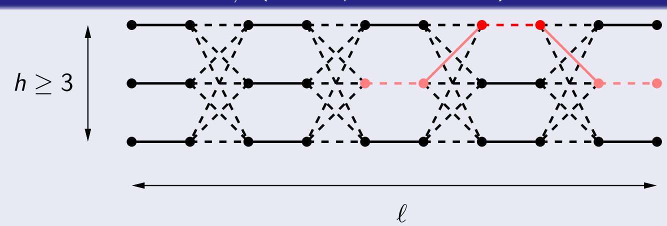


Augmenting path

Worst-case graph $G_{h,\ell}$ (Sasaki/Hajek, 1988)



Augmenting path can get shorter

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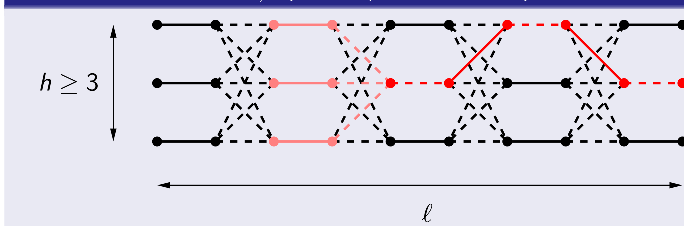

Augmenting path can get shorter but is more likely to get longer.

Theorem

For $h \geq 3$, the (1+1) EA has exponential expected runtime $2^{\Omega(\ell)}$ on $G_{h,\ell}$.

Proof by drift analysis

(1+1) EA for the Maximum Matching Problem
(1+1) EA is a PRAS

Insight: do not hope for exact solutions but for approximations

Theorem (Giel/Wegener, 2003)

For $\varepsilon > 0$, the (1+1) EA finds a $(1+\varepsilon)$-approximation of a maximum matching in expected time $O(m^{2\lceil 1/\varepsilon \rceil})$ and is a polynomial-time randomized approximation scheme (PRAS).

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Proof idea:

- Look into the analysis of the Hopcroft/Karp algorithm.
- Current solution worse than $(1+\varepsilon)$-approximate $\rightarrow$ many augmenting paths, in partic. a short one of length $\leq 2\lceil \varepsilon^{-1} \rceil$
- Wait for the (1+1) EA to optimize this short path.

Agenda

(1+1) EA and the Partition Problem

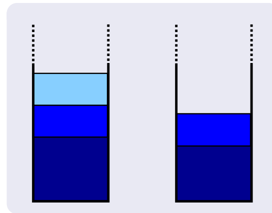
What about NP-hard problems? $\rightarrow$ Study approximation quality

(1+1) EA and the Partition Problem

What about NP-hard problems? → Study approximation quality

For $w_1, \dots, w_n$, find $I \subseteq \{1, \dots, n\}$ minimizing

$$\max\left\{\sum_{i \in I} w_i, \sum_{i \notin I} w_i\right\}.$$



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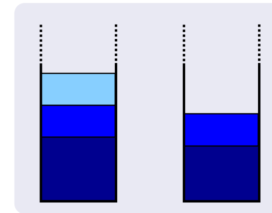

This is an "easy" NP-hard problem:

- not strongly NP-hard,
- FPTAS exist,
- ...

(1+1) EA for the Partition Problem
Worst-Case Results

Coding: bit string $\{0,1\}^n$ encodes I

Fitness function: weight of fuller bin

Theorem (Witt, 2005)

On any instance for the partition problem, the (1+1) EA reaches a solution with approximation ratio $4/3$ *in expected time* $O(n^2)$.

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Theorem

There is an instance such that the (1+1) EA needs with prob. $\Omega(1)$ *at least* $n^{\Omega(n)}$ *steps to find a solution with a better ratio than* $4/3 - \varepsilon$.

Proof ideas: study effect of local steps and local optima

(1+1) EA for the Partition Problem
Worst Case – PRAS by Parallelism

Theorem

On any instance, the (1+1) EA with prob. $\geq 2^{-c\lceil 1/\varepsilon\rceil \ln(1/\varepsilon)}$ finds a $(1+\varepsilon)$-approximation within $O(n\ln(1/\varepsilon))$ steps.

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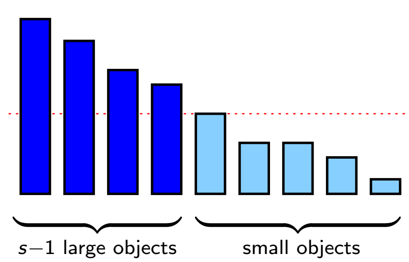
- $2^{O(\lceil 1/\varepsilon\rceil \ln(1/\varepsilon))}$ parallel runs find a $(1+\varepsilon)$-approximation with prob. $\geq 3/4$ in $O(n\ln(1/\varepsilon))$ parallel steps.
- Parallel runs form a PRAS!

(1+1) EA for the Partition Problem
Worst Case – PRAS by Parallelism (Proof Idea)

Set $s := \lceil \frac{2}{\varepsilon} \rceil$ and $w := \sum_{i=1}^{n} w_i$.

Assuming $w_1 \geq \cdots \geq w_n$, we have $w_i \leq \varepsilon \frac{w}{2}$ for $i \geq s$.



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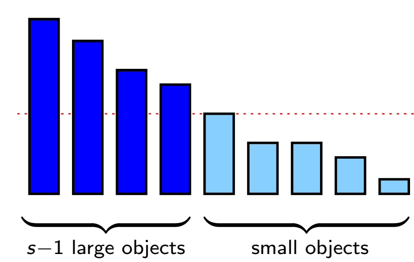

Analyze probability of distributing

- large objects in an optimal way,
- small objects greedily $\Rightarrow$ additive error $\leq \varepsilon w/2$,

This is the algorithmic idea by Graham (1969).

(1+1) EA for the Partition Problem
Average-Case Analyses

Models: each weight drawn independently at random, namely

1. uniformly from the interval $[0, 1]$,
2. exponentially distributed with parameter 1 (i. e., $\text{Prob}(X \geq t) = e^{-t}$ for $t \geq 0$).

Approximation ratio no longer meaningful, we investigate:
discrepancy = absolute difference between weights of bins.

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How close to discrepancy 0 do we come?

(1+1) EA for the Partition Problem
Partition Problem - Known Averge-Case Results

Deterministic, problem-specific heuristic LPT

Sort weights decreasingly,
put every object into currently emptier bin.

Analysis in both random models:

After LPT has been run, additive error is $O((\log n)/n)$ (Frenk/Rinnooy Kan, 1986).

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Can RLS or the (1+1) EA reach a discrepancy of $o(1)$?

(1+1) EA for the Partition Problem
New Result

Theorem

In both models, the (1+1) EA reaches discrepancy $O((\log n)/n)$ after $O(n^{c+4} \log^2 n)$ steps with probability $1 - O(1/n^c)$.

Almost the same result as for LPT!

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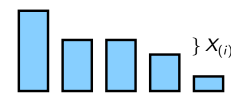
Proof exploits order statistics:

W. h. p.
$X_{(i)} - X_{(i+1)} = O((\log n)/n)$
for $i = \Omega(n)$.



Agenda

Simulated Annealing Beats Metropolis in Combinatorial Optimization

Jerrum/Sinclair (1996)

"It remains an outstanding open problem to exhibit a natural example in which simulated annealing with any non-trivial cooling schedule provably outperforms the Metropolis algorithm at a carefully chosen fixed value" of the temperature.

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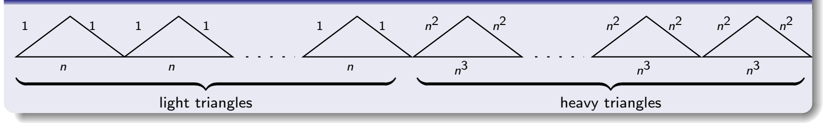
Solution (Wegener, 2005): MSTs are such an example.

A bad instance for MA



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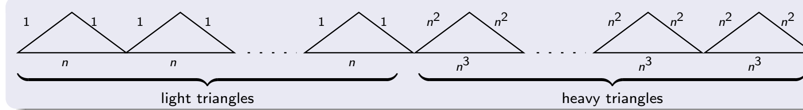

Theorem (Wegener, 2005)

The MA with arbitrary temperature computes the MST for this instance only with probability $e^{-\Omega(n)}$ in polynomial time. SA with temperature $T_t := n^3(1-\Theta(1/n))^t$ computes the MST in $O(n \log n)$ steps with probability $1 - O(1/poly(n))$.

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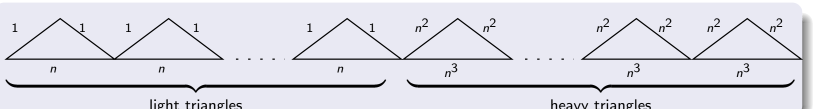

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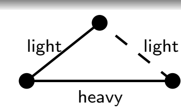
Proof idea: need different temperatures to optimize all triangles.

Simulated Annealing Beats Metropolis in Combinatorial Optimization

Proof Idea

Concentrate on wrong triangles:
one heavy, one light edge chosen



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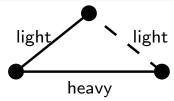

- Soon after initialization $\Omega(n)$ wrong triangles, both in heavy and light part of the graph
- To correct such triangle, light edge must be flipped in.

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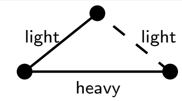

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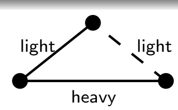

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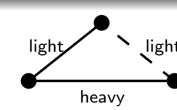

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- Light edges of heavy triangles still much heavier than heavy edges of light triangles $\rightarrow$ at temperature T^* almost random search on light triangles $\rightarrow$ many light triangles remain wrong.
- SA first corrects heavy triangles at temperature T^*.
- After temperature has dropped, SA corrects light triangles, without destroying heavy ones.

Summary and Conclusions

- Analysis of RSHs in combinatorial optimization
- Starting from toy problems to real problems
- Surprising results
- Interesting techniques
- Analysis of new approaches

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→ Altogether, an exciting research direction.

Suggested Reading

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Theory of Randomized Search Heuristics – Foundations and Recent Developments, World Scientific Publishing, 2011

Frank Neumann, Carsten Witt:
Bio-Inspired Computation in Combinatorial Optimization – Algorithms and Their Computational Complexity, Springer, 2010
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Thank you!