



Bioinspired computation in combinatorial optimization - Algorithms and their computational complexity

Neumann, Frank; Witt, Carsten

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Bioinspired Computation in Combinatorial Optimization – Algorithms and Their Computational Complexity

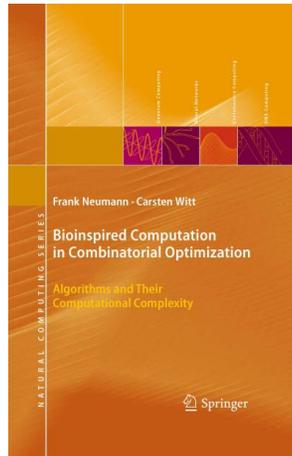
Frank Neumann¹ Carsten Witt²

¹The University of Adelaide
cs.adelaide.edu.au/~frank

²Technical University of Denmark
www.imm.dtu.dk/~cawi

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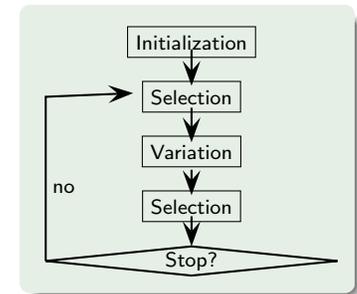


Book available at www.bioinspiredcomputation.com 1/88

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"
- actually it's only an algorithm, a **randomized search heuristic (RSH)**



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

$$\text{Optimize } f: \{0, 1\}^n \rightarrow \mathbb{R}$$

Why Do We Consider Randomized Search Heuristics?

- Not enough resources (time, money, knowledge) for a tailored algorithm
- Black Box Scenario $x \rightarrow \text{[Box]} \rightarrow f(x)$ rules out problem-specific algorithms
- We like the simplicity, robustness, ... of Randomized Search Heuristics
- They are surprisingly successful.

Point of view

Want 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)
- 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 and RLS 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 $x_{t+1} := x_t$.

RLS

- 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 $x_{t+1} := x_t$.

5/88

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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

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

6/88

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How Do We Obtain Results?

We use (rarely in their pure form):

- Coupon Collector's Theorem
- 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, martingale theory, electrical networks
- Random graphs (esp. random trees)
- Identifying typical events and failure events
- Potential functions and amortized analysis
- ...

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

7/88

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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
- ...

High-quality results, but limited to SA/MA (nothing about EAs) and hard to generalize.

Since the early 1990s

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

8/88

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This Tutorial

- 1 The origins: example functions and toy problems
 - A simple toy problem: OneMax for (1+1) EA
- 2 Combinatorial optimization problems
 - Minimum spanning trees
 - Maximum matchings
 - Shortest paths
 - Makespan scheduling
 - Covering problems
 - Traveling salesman problem
- 3 End
- 4 References

9/88

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

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 ...

10/88

Agenda

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- 3 End
- 4 References

11/88

Example: OneMax

Theorem (e. g., Droste/Jansen/Wegener, 1998)

The expected runtime of the RLS, (1+1) EA, ($\mu+1$) EA, (1+ λ) EA on ONEMAX is $\Omega(n \log n)$.

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 ($\mu+1$) EA and for (1+ λ) EA with small populations.

12/88

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

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

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

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

13/88

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 \rightarrow Real Royal Road Functions
- multistarts vs. populations
- frequent restarts vs. long runs
- dynamic schedules
- ...

14/88

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 salesman problem,
 - Eulerian cycles,
 - minimum spanning trees,
 - maximum matchings,
 - scheduling problems,
 - shortest paths,
 - ...
- We do not hope: to be better than the best problem-specific algorithms
- Instead: maybe reasonable polynomial running times
- In the following no fine-tuning of the results

15/88

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- 4 References

16/88

Minimum Spanning Trees:

- **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.
- Search space $\{0,1\}^m$
- Edge e_i is chosen iff $x_i=1$
- Consider (1+1) EA

17/88

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.

18/88

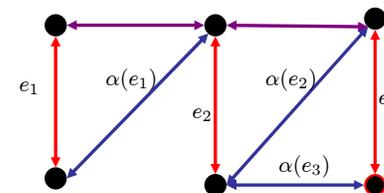
First goal: Obtain a connected subgraph of G .

How long does it take?

Connected graph in expected time $O(m \log n)$
(fitness-based partitions)

19/88

Bijection for minimum spanning trees:



$k := |E(T^*) \setminus E(T)|$
 Bijection $\alpha: E(T^*) \setminus E(T) \rightarrow E(T) \setminus E(T^*)$
 $\alpha(e_i)$ on the cycle of $E(T) \cup \{e_i\}$
 $w(e_i) \leq w(\alpha(e_i))$
 $\Rightarrow k$ accepted 2-bit flips that turn T into T^*

20/88

Upper Bound

Theorem:

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 .
- w_{opt} weight minimum spanning tree T^*
- set of $m + 1$ operations to reach T^*
- $m' = m - (n - 1)$ 1-bit flips concerning non- T^* edges \Rightarrow spanning tree T
- k 2-bit flips defined by bijection
- $n - k$ non accepted 2-bit flips
- \Rightarrow average distance decrease $(w(s) - w_{\text{opt}})/(m + 1)$

21/88

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Proof

1-step (larger total weight decrease of 1-bit flips)

2-step (larger total weight decrease of 2-bit flips)

Consider 2-steps:

- Expected weight decrease by a factor $1 - (1/(2n))$
- Probability (n/m^2) for a good 2-bit flip
- Expected time until q 2-steps $O(qm^2/n)$

Consider 1-steps:

- Expected weight decrease by a factor $1 - (1/(2m'))$
- Probability (m'/m) for a good 1-bit flip
- Expected time until q 1-steps $O(qm/m')$

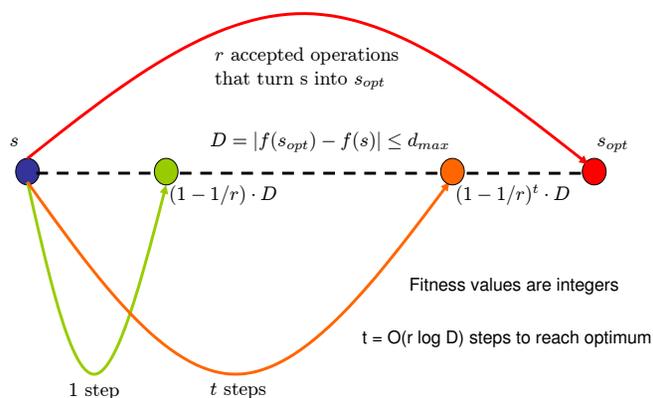
1-steps faster \Rightarrow show bound for 2-steps.

22/88

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Expected Multiplicative Distance Decrease (aka Drift Analysis)



23/88

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Maximum distance: $w(s) - w_{\text{opt}} \leq D := m \cdot w_{\max}$

1 step: Expected distance at most $(1 - 1/(2n))(w(s) - w_{\text{opt}})$

t steps: Expected distance at most $(1 - 1/(2n))^t (w(s) - w_{\text{opt}})$

$t := \lceil 2 \cdot (\ln 2)n(\log D + 1) \rceil$: $(1 - 1/(2n))^t (w(s) - w_{\text{opt}}) \leq 1/2$

Expected number of 2-steps $2t = O(n(\log n + \log w_{\max}))$ (Markov)

Expected optimization time

$O(tm^2/n) = O(m^2(\log n + \log w_{\max}))$.

24/88

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 - Covering problems
 - Traveling salesman problem
- 3 End
- 4 References

25/88

Maximum Matchings

A **matching** in an undirected graph is a subset of pairwise disjoint edges;
aim: find a maximum matching (solvable in poly-time)

Simple example: path of odd length



Maximum matching with more than half of edges

26/88

Maximum Matchings

A **matching** in an undirected graph is a subset of pairwise disjoint edges;
aim: find a maximum matching (solvable in poly-time)

Simple example: path of odd length



Suboptimal matching

Concept: augmenting path

- Alternating between edges being inside and outside the matching
- Starting and ending at "free" nodes not incident on matching
- Flipping all choices along the path improves matching

Example: whole graph is augmenting path

Interesting: how simple EAs find augmenting paths

26/88

Maximum Matchings: Upper Bound

Fitness function $f: \{0, 1\}^{\# \text{ edges}} \rightarrow \mathbb{R}$:

- one bit for each edge, value 1 iff edge chosen
- value for legal matchings: size of matching
- otherwise penalty leading to empty matching

Example: path with $n + 1$ nodes, n edges: bit string selects edges



Theorem

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

27/88

Maximum Matchings: Upper Bound (Ctnd.)

Proof idea for $O(n^4)$ bound

- Consider the level of second-best matchings.
- Fitness value does not change (walk on *plateau*).
- If “free” edge: chance to flip one bit! → probability $\Theta(1/n)$.
- Else steps flipping two bits → probability $\Theta(1/n^2)$.
- Shorten or lengthen augmenting path
- At length 1, chance to flip the free edge!



- Length changes according to a **fair random walk**
→ equal probability for lengthenings and shortenings

28/88

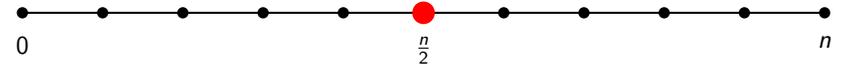
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Fair Random Walk

Scenario: fair random walk

- Initially, player *A* and *B* both have $\frac{n}{2}$ USD
- Repeat: flip a coin
- If heads: *A* pays 1 USD to *B*, tails: other way round
- Until one of the players is ruined.



How long does the game take in expectation?

Theorem:

Fair random walk on $\{0, \dots, n\}$ takes in expectation $O(n^2)$ steps.

29/88

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Maximum Matchings: Upper Bound (Ctnd.)

Proof idea for $O(n^4)$ bound

- Consider the level of second-best matchings.
- Fitness value does not change (walk on *plateau*).
- If “free” edge: chance to flip one bit! → probability $\Theta(1/n)$.
- Else steps flipping two bits → probability $\Theta(1/n^2)$.
- Shorten or lengthen augmenting path
- At length 1, chance to flip the free edge!



Length changes according to a **fair random walk**, expected $O(n^2)$ two-bit flips suffice, expected optimization time $O(n^2) \cdot O(n^2) = O(n^4)$.

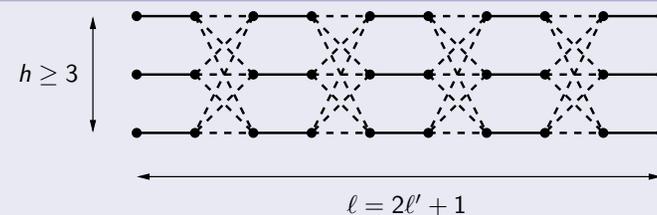
30/88

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Maximum Matchings: Lower Bound

Worst-case graph $G_{h,\ell}$



Augmenting path can get shorter **but is more likely to get longer.**
(**unfair** random walk)

Theorem

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

Proof requires analysis of negative drift (simplified drift theorem).

31/88

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Insight: do not hope for exact solutions but for approximations

For maximization problems: solution with value a is called $(1 + \varepsilon)$ -approximation if $\frac{OPT}{a} \leq 1 + \varepsilon$, where OPT optimal value.

Theorem

For $\varepsilon > 0$, $(1+1)$ EA finds a $(1 + \varepsilon)$ -approximation of a maximum matching in expected time $O(m^{2/\varepsilon+2})$ (m number of edges).

Proof idea: If current solution worse than $(1 + \varepsilon)$ -approximate, there is a "short" augmenting path (length $\leq 2/\varepsilon + 1$); flip it in one go.

32/88

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- 3 End
- 4 References

33/88

All-pairs-shortest-path (APSP) problem

Given: Connected directed graph $G = (V, E)$, $|V| = n$ and $|E| = m$, and a function $w: E \rightarrow \mathbb{N}$ which assigns positive integer weights to the edges.

Compute from each vertex $v_i \in V$ a shortest path (path of minimal weight) to every other vertex $v_j \in V \setminus \{v_i\}$

Representation:

Individuals are paths between two particular vertices v_i and v_j

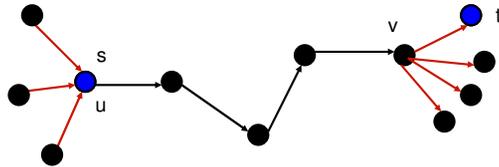
Initial Population: $P := \{I_{u,v} = (u, v) \mid (u, v) \in E\}$

Mutation-based EA

Mutation:

Pick individual $I_{u,v}$ uniformly at random

$E^-(u)$: incoming edges of u $E^+(v)$: outgoing edges of v



Pick uniformly at random an edge $e = (x, y) \in E^-(u) \cup E^+(v)$

Add e New individual $I'_{s,t}$

Steady State EA

1. Set $P = \{I_{u,v} = (u, v) \mid (u, v) \in E\}$.
2. Choose an individual $I_{x,y} \in P$ uniformly at random.
3. Mutate $I_{x,y}$ to obtain an individual $I'_{s,t}$.
4. If there is no individual $I_{s,t} \in P$, $P = P \cup \{I'_{s,t}\}$, else if $f(I'_{s,t}) \leq f(I_{s,t})$, $P = (P \cup \{I'_{s,t}\}) \setminus \{I_{s,t}\}$
5. Repeat Steps 2-4 forever.

Lemma:

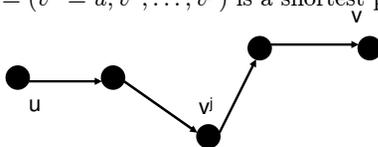
Let $\ell \geq \log n$. The expected time until has found all shortest paths with at most ℓ edges is $O(n^3 \ell)$.

Proof idea:

Consider two vertices u and v , $u \neq v$.

Let $\gamma := (v^1 = u, v^2, \dots, v^{\ell+1} = v)$ be a shortest path from u to v consisting of ℓ' , $\ell' \leq \ell$, edges in G

the sub-path $\gamma' = (v^1 = u, v^2, \dots, v^j)$ is a shortest path from u to v^j .



(E. 2018-1)

Population size is upper bounded n^2
(for each pair of vertices at most one path)

- Pick shortest path from u to v_j and append edge (v_j, v_{j+1})
- Shortest path from u to v_{j+1}
- Probability to pick I_{u,v_j} is at least $1/n^2$
- Probability to append right edge is at least $1/(2n)$
- **Success** with probability at least $p = 1/(2n^3)$
- **At most 1 successes needed** to obtain shortest path from u to v

Analysis

Consider typical run consisting of $T=cn^3l$ steps.

What is the probability that the shortest path from u to v has been obtained?

We need at most l successes, where a success happens in each step with probability at least $p = 1/(2n^3)$

Define for each step i a random variable X_i .

$X_i = 1$ if step i is a success

$X_i = 0$ if step i is not a success

$$Prob(X_i = 1) \geq p = 1/(2n^3) \quad X = \sum_{i=1}^T X_i \quad X \geq l \text{ ???}$$

$$\text{Expected number of successes } E(X) \geq T/(2n^3) = \frac{cn^3l}{2n^3} = \frac{cl}{2}$$

$$\text{Chernoff: } Prob(X < (1 - \delta)E(x)) \leq e^{-E(X)\delta^2/2}$$

$$\delta = \frac{1}{2}$$

$$Prob(X < (1 - \frac{1}{2})E(x)) \leq e^{-E(X)/8} \leq e^{-T/(16n^3)} = e^{-cn^3l/(16n^3)} = e^{-cl/(16)}$$

$$\text{Probability for failure of at least one pair of vertices at most: } n^2 \cdot e^{-cl/16}$$

c large enough and $l \geq \log n$:

$$\text{No failure in any path with probability at least } \alpha = 1 - n^2 \cdot e^{-cl/16} = 1 - o(1)$$

Holds for any phase of T steps

$$\text{Expected time upper bound by } T/\alpha = O(n^3l)$$

Shortest paths have length at most $n-1$.

Set $l = n-1$

Theorem

The expected optimization time of Steady State EA for the APSP problem is $O(n^4)$.

Remark:

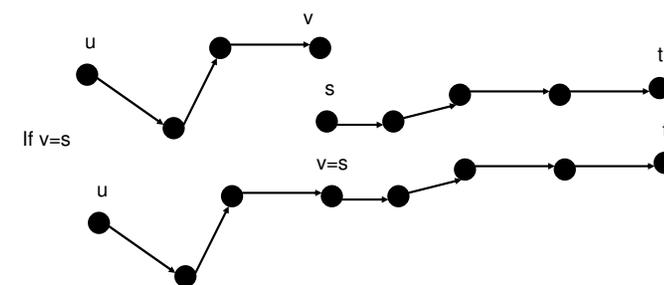
There are instances where the expected optimization of $(\mu + 1)$ -EA is $\Omega(n^4)$

Question:

Can crossover help to achieve a better expected optimization time?

Crossover

Pick two individuals $I_{u,v}$ and $I_{s,t}$ from population uniformly at random.



Steady State GA

1. Set $P = \{I_{u,v} = (u,v) \mid (u,v) \in E\}$.
2. Choose $r \in [0, 1]$ uniformly at random.
3. If $r \leq p_c$, choose two individuals $I_{x,y} \in P$ and $I_{x',y'} \in P$ uniformly at random and perform crossover to obtain an individual $I'_{s,t}$, else choose an individual $I_{x,y} \in P$ uniformly at random and mutate $I_{x,y}$ to obtain an individual $I'_{s,t}$.
4. If $I'_{s,t}$ is a path from s to t then
 - ★ If there is no individual $I_{s,t} \in P$, $P = P \cup \{I'_{s,t}\}$,
 - ★ else if $f(I'_{s,t}) \leq f(I_{s,t})$, $P = (P \cup \{I'_{s,t}\}) \setminus \{I_{s,t}\}$.
5. Repeat Steps 2-4 forever.

p_c is a constant

Theorem:

The expected optimization time of Steady State GA is $O(n^{3.5} \sqrt{\log n})$.

Mutation and $\ell^* := \sqrt{n \log n}$

All shortest path of length at most ℓ^* edges are obtained

Show: Longer paths are obtained by crossover within the stated time bound.

Analysis Crossover

Long paths by crossover:

Assumption: All shortest paths with at most ℓ^* edges have already been obtained.

Assume that all shortest paths of length $k \leq \ell^*$ have been obtained.

What is the expected time to obtain all shortest paths of length at most $3k/2$?

Analysis Crossover

Consider pair of vertices x and y for which a shortest path of length r , $k < r \leq 3k/2$, exists.

There are $2k-r$ pairs of shortest paths of length at most k that can be joined to obtain shortest path from x to y .

Probability for one specific pair: at least $1/n^4$

At least $2k+1-r$ possible pairs: probability at least $(2k+1-r)/n^4 \geq k/(2n^4)$

At most n^2 shortest paths of length r , $k < r \leq 3k/2$

Time to collect all paths $O(n^4 \log n/k)$
(similar to Coupon Collectors Theorem)

Analysis Crossover

Sum up over the different values of k , namely

$$\sqrt{n \log n}, c \cdot \sqrt{n \log n}, c^2 \cdot \sqrt{n \log n}, \dots, c^{\log_c(n/\sqrt{n \log n})} \cdot \sqrt{n \log n},$$

where $c = 3/2$.

Expected Optimization

$$\sum_{s=0}^{\log_c(n/\sqrt{n \log n})} \left(O\left(\frac{n^4 \log n}{\sqrt{n \log n}}\right) c^{-s} \right) = O(n^{3.5} \sqrt{\log n}) \sum_{s=0}^{\infty} c^{-s} = O(n^{3.5} \sqrt{\log n})$$

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- 4 References

Makespan Scheduling

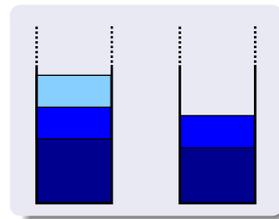
What about NP-hard problems? → Study approximation quality

Makespan scheduling on 2 machines:

- n objects with weights/processing times w_1, \dots, w_n
- 2 machines (bins)
- Minimize the total weight of fuller bin = makespan.

Formally, find $I \subseteq \{1, \dots, n\}$ minimizing

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



Sometimes also called the **Partition** problem.

This is an “easy” NP-hard problem, good approximations possible

Fitness Function

- Problem encoding: bit string x_1, \dots, x_n reserves a bit for each object, put object i in bin $x_i + 1$.
- Fitness function

$$f(x_1, \dots, x_n) := \max \left\{ \sum_{i=1}^n w_i x_i, \sum_{i=1}^n w_i (1 - x_i) \right\}$$

to be minimized.

- Consider (1+1) EA and RLS.

Types of Results

- Worst-case results
- Success probabilities and approximations
- An average-case analysis
- A parameterized analysis

52/88

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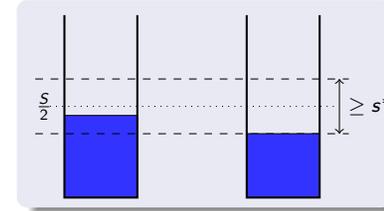
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Sufficient Conditions for Progress

Abbreviate $S := w_1 + \dots + w_n \Rightarrow$ perfect partition has cost $\frac{S}{2}$.

Suppose we know

- s^* = size of smallest object in the fuller bin,
 - $f(x) > \frac{S}{2} + \frac{s^*}{2}$ for the current search point x
- then the solution is improvable by a single-bit flip.



If $f(x) < \frac{S}{2} + \frac{s^*}{2}$, no improvements can be guaranteed.

Lemma

If smallest object in fuller bin is always bounded by s^ then $(1+1)$ EA and RLS reach f -value $\leq \frac{S}{2} + \frac{s^*}{2}$ in expected $O(n^2)$ steps.*

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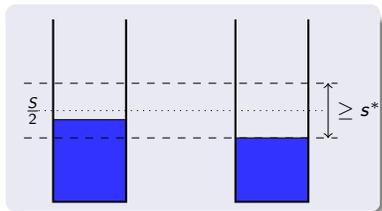
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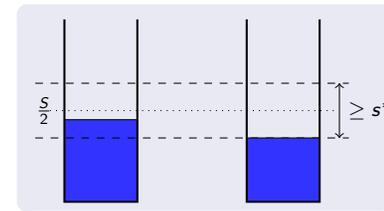
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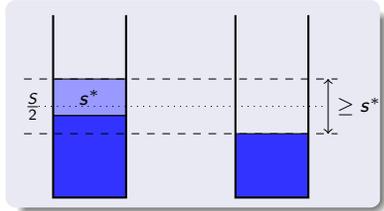
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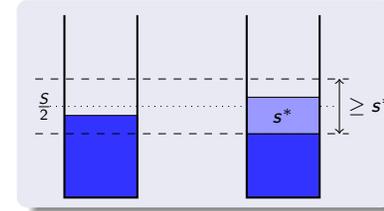
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53/88

Worst-Case Results

Theorem

On any instance to the makespan scheduling problem, the $(1+1)$ EA and RLS reach a solution with approximation ratio $\frac{4}{3}$ in expected time $O(n^2)$.

Use study of object sizes and previous lemma.

Theorem

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

54/88

Worst-Case Instance

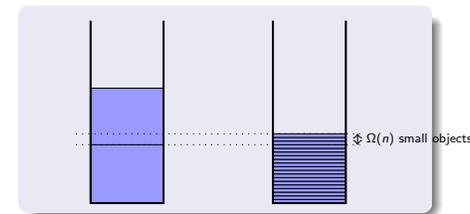
Instance $W_\epsilon^* = \{w_1, \dots, w_n\}$ is defined by $w_1 := w_2 := \frac{1}{3} - \frac{\epsilon}{4}$ (big objects) and $w_i := \frac{1/3 + \epsilon/2}{n-2}$ for $3 \leq i \leq n$, ϵ very small constant; n even

Sum is 1; there is a perfect partition.

But if one bin with big and one bin with small objects: value $\frac{2}{3} - \frac{\epsilon}{2}$.

Move a big object in the emptier bin \Rightarrow value $(\frac{1}{3} + \frac{\epsilon}{2}) + (\frac{1}{3} - \frac{\epsilon}{4}) = \frac{2}{3} + \frac{\epsilon}{4}$!

Need to move $\geq \epsilon n$ small objects at once for improvement: very unlikely.



With constant probability in this situation, $n^{\Omega(n)}$ needed to escape.

55/88

Worst Case – PRAS by Parallelism

Previous result shows: success dependent on big objects

Theorem

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

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

56/88

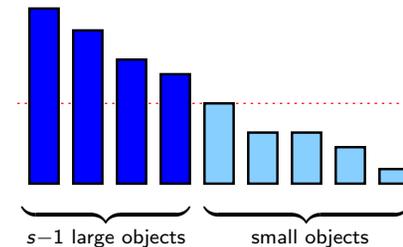
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Worst Case – PRAS by Parallelism (Proof Idea)

Set $s := \lceil \frac{2}{\varepsilon} \rceil$

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



analyze probability of distributing

- large objects in an optimal way,
- small objects greedily \Rightarrow error $\leq \varepsilon \frac{S}{2}$,

Random search rediscovers algorithmic idea of early algorithms.

57/88

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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.

How close to discrepancy 0 do we come?

58/88

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Makespan Scheduling – Known Average-Case Results

Deterministic, problem-specific heuristic LPT

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

Known for both random models:

LPT creates a solution with discrepancy $O((\log n)/n)$.

What discrepancy do the (1+1) EA and RLS reach in poly-time?

59/88

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Average-Case Analysis of the (1+1) EA

Theorem

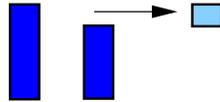
In both models, the (1+1) EA reaches discrepancy $O((\log n)/n)$ after $O(n^{c+4} \log^2 n)$ steps with probability $1 - O(1/n^c)$.

Almost the same result as for LPT!

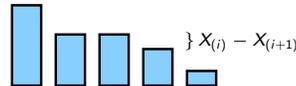
Proof exploits order statistics:

If $X_{(i)}$ (i -th largest) in fuller bin, $X_{(i+1)}$ in emptier one, and discrepancy $> 2(X_{(i)} - X_{(i+1)}) > 0$, then objects can be swapped; discrepancy falls

Consider such “difference objects”.



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



60/88

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A Parameterized Analysis

Have seen: problem is hard for (1+1) EA/RLS in the worst case, but not so hard on average.

What **parameters** make the problem hard?

Definition

A problem is *fixed-parameter tractable (FPT)* if there is a problem parameter k such that it can be solved in time $f(k) \cdot \text{poly}(n)$, where $f(k)$ does not depend on n .

Intuition: for small k , we have an efficient algorithm.

Considered parameters (Sutton and Neumann, 2012):

- 1 Value of optimal solution
- 2 No. jobs on fuller machine in optimal solution
- 3 Unbalance of optimal solution

61/88

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Value of Optimal Solution

Recall **approximation** result: decent chance to distribute k big jobs optimally if k small.

Since $w_1 \geq \dots \geq w_n$, already $w_k \leq S/k$.

Consequence: optimal distribution of first k objects \rightarrow can reach makespan $S/2 + S/k$ by greedily treating the other objects.

Theorem

(1+1) EA and RLS find solution of makespan $\leq S/2 + S/k$ with probability $\Omega((2k)^{-ek})$ in time $O(n \log k)$. Multistarts have success probability $\geq 1/2$ after $O(2^{(e+1)k} k^{ek} n \log k)$ evaluations.

$2^{(e+1)k} k^{ek} \log k$ does not depend on $n \rightarrow$ a **randomized FPT-algorithm**.

62/88

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No. Objects on Fuller Machine

Suppose: optimal solution puts only k objects on fuller machine.
Notion: k is called *critical path size*.

Intuition:

- Good chance of putting k objects on same machine if k small,
- other objects can be moved greedily.

Theorem

For critical path size k , multistart RLS finds optimum in $O(2^k (en)^{ck} n \log n)$ evaluations with probability $\geq 1/2$.

Due to term n^{ck} , result is somewhat weaker than FPT (a so-called XP-algorithm). Still, for constant k polynomial.

Remark: with (1+1)-EA, get an additional $\log w_1$ -term.

63/88

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Unbalance of Optimal Solution

Consider **discrepancy** of optimum $\Delta^* := 2(\text{OPT} - S/2)$.

Question/decision problem: Is $w_k \geq \Delta^* \geq w_{k+1}$?

Observation: If $\Delta^* \geq w_{k+1}$, optimal solution will put w_{k+1}, \dots, w_n on emptier machine. Crucial to distribute first k objects optimally.

Theorem

Multistart RLS with biased mutation (touches objects w_1, \dots, w_k with prob. $1/(kn)$ each) solves decision problem in $O(2^k n^3 \log n)$ evaluations with probability $\geq 1/2$.

Again, a randomized FPT-algorithm.

64/88

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Agenda

- 1 The origins: example functions and toy problems
 - A simple toy problem: OneMax for (1+1) EA
- 2 Combinatorial optimization problems
 - Minimum spanning trees
 - Maximum matchings
 - Shortest paths
 - Makespan scheduling
 - Covering problems
 - Traveling salesman problem
- 3 End
- 4 References

65/88

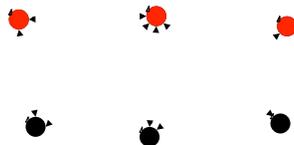
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The Problem

The Vertex Cover Problem:

Given an undirected graph $G=(V,E)$.



Find a minimum subset of vertices such that each edge is covered at least once.

NP-hard, several 2-approximation algorithms.

Simple single-objective evolutionary algorithms fail!!!

66/88

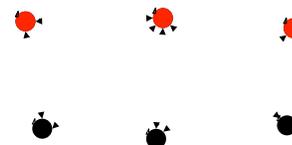
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The Problem

Integer Linear Program (ILP)

$$\begin{aligned} \min \sum_{i=1}^n x_i \\ \text{s.t. } x_i + x_j \geq 1 \quad \forall \{i, j\} \in E \\ x_i \in \{0, 1\} \end{aligned}$$



Linear Program (LP)

$$\begin{aligned} \min \sum_{i=1}^n x_i \\ \text{s.t. } x_i + x_j \geq 1 \quad \forall \{i, j\} \in E \\ x_i \in [0, 1] \end{aligned}$$

Decision problem: Is there a set of vertices of size at most k covering all edges?

Our parameter: Value of an optimal solution (OPT)

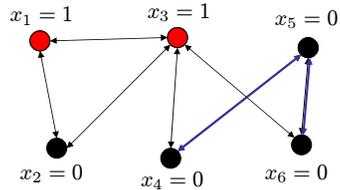
67/88

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Evolutionary Algorithm

Representation: Bitstrings of length n



Minimize fitness function:

$$f_1(x) = (|x|_1, |U(x)|)$$

$$f_1(x) = (2, 2)$$

$$f_2(x) = (|x|_1, LP(x))$$

$$f_2(x) = (2, 1)$$

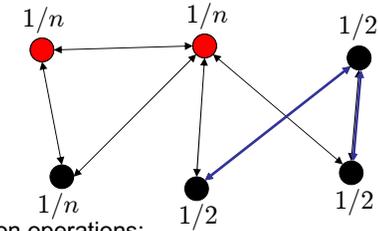
$U(x)$: Edges not covered by x

$$G(x) = G(V, U(x))$$

$LP(x)$: value of LP applied to $G(x)$

68/88

Evolutionary Algorithm



Two mutation operations:

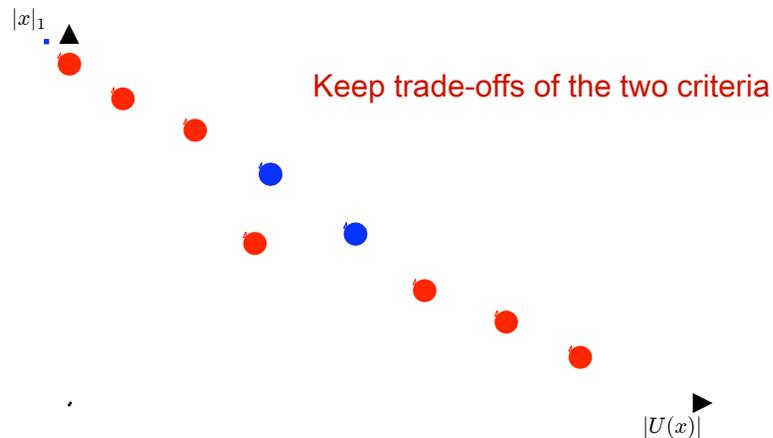
1. Standard bit mutation with probability $1/n$
2. Mutation probability $1/2$ for vertices adjacent to edges of $U(x)$.
Otherwise mutation probability $1/n$.

Decide uniformly at random which operator to use in next iteration

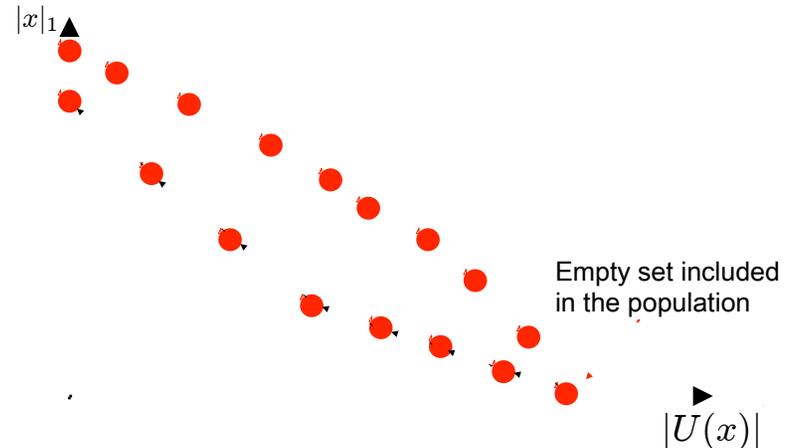
69/88

Multi-Objective Approach:

Treat the different objectives in the same way

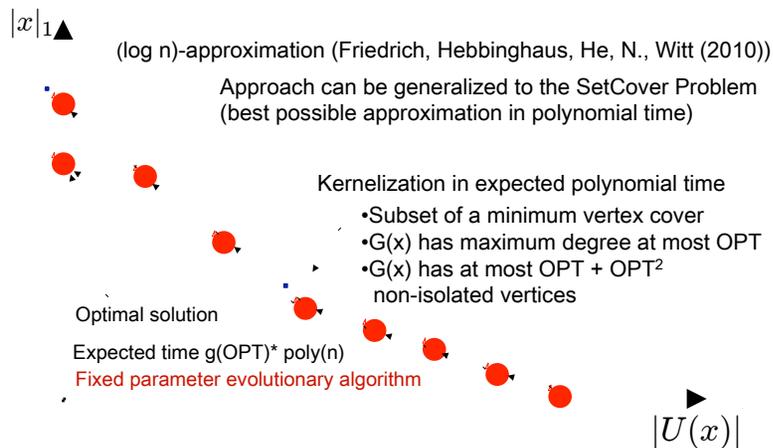


70/88

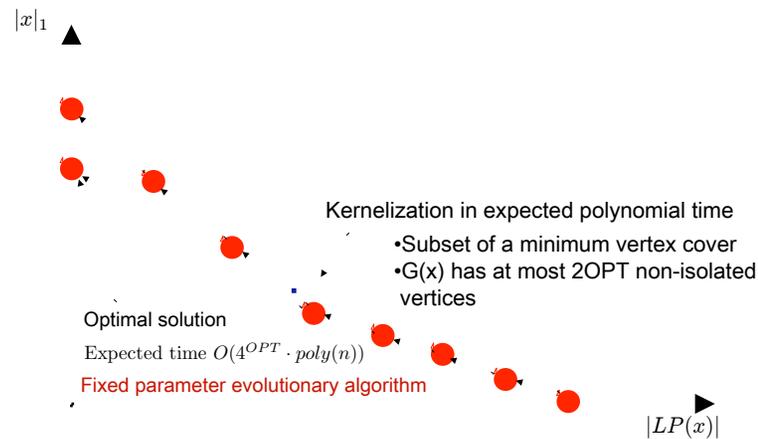


71/88

What can we say about these solutions?



72/88



73/88

Linear Programming

Combination with Linear Programming

- LP-relaxation is half integral, i.e.

$$x_i \in \{0, 1/2, 1\}, 1 \leq i \leq n$$

Theorem (Nemhauser, Trotter (1975)):

Let x^* be an optimal solution of the LP. Then there is a minimum vertex cover that contains all vertices v_i where $x_i^* = 1$.

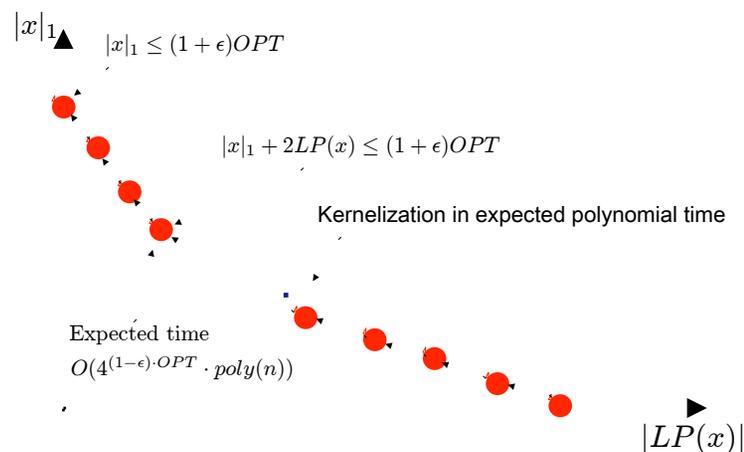
Lemma:

All search points x with $LP(x) = LP(0^n) - |x|_1$ are Pareto optimal. They can be extended to minimum vertex cover by selecting additional vertices.

Can we also say something about approximations?

74/88

Approximations



75/88

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76/88

Euclidean TSP

Given n points in the plane and Euclidean distances between the cities.

Find a shortest tour that visits each city exactly once and return to the origin.

NP-hard, PTAS, **FPT when number of inner points is the parameter.**

77/88

Representation and Mutation

Representation: Permutation of the n cities

For example: (3, 4, 1, 2, 5)

Inversion (inv) as mutation operator:

- Select i, j from $\{1, \dots, n\}$ uniformly at random and invert the part from position i to position j .
- Inv(2,5) applied to (3, 4, 1, 2, 5) yields (3, 5, 2, 1, 4)

78/88

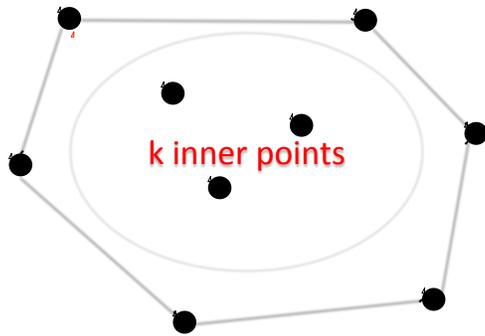
(1+1) EA

```
 $x \leftarrow$  a random permutation of  $[n]$ .  
repeat forever  
   $y \leftarrow$  MUTATE( $x$ )  
  if  $f(y) < f(x)$  then  $x \leftarrow y$ 
```

Mutation:

(1+1) EA: k random inversion,
 k chosen according to
1+Pois(1)

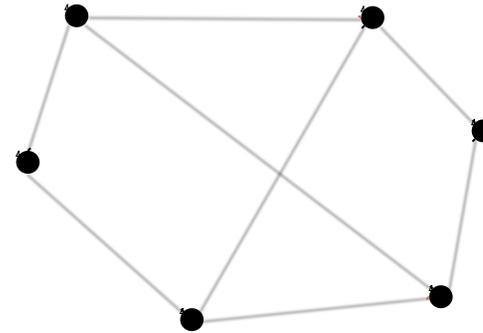
79/88



Convex hull containing n-k points

80/88

Intersection and Mutation



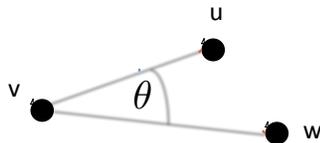
81/88

Angle bounded set of points

There may be an exponential number of inversion to end up in a local optimum if points are in arbitrary positions (Englert et al, 2007).

We assume that the set V is angle bounded

V is *angle-bounded* by $\epsilon > 0$ if for any three points $u, v, w \in V$, $0 < \epsilon < \theta < \pi - \epsilon$ where θ denotes the angle formed by the line from u to v and the line from v to w .



If V is angle-bounded then we get a lower bound on an improvement depending on ϵ

82/88

Progress

Assumptions:

d_{\max} : Maximum distance between any two points

d_{\min} : Minimum distance between any two points

V is angle-bounded by ϵ

Whenever the current tour is not intersection-free, we can guarantee a certain progress

Lemma:

Let x be a permutation such that is not intersection-free. Let y be the permutation constructed from an inversion on x that replaces two intersecting edges with two non-intersecting edges. Then, $f(x) - f(y) > 2d_{\min} \left(\frac{1 - \cos(\epsilon)}{\cos(\epsilon)} \right)$.

83/88

Tours

A tour x is either

- Intersection free
- Non intersection free

Intersection free tours are good. The points on the convex hull are already in the right order (Quintas and Supnick, 1965).

Claim: We do not spend too much time on non intersection free tours.

Time spend on intersecting tours

Lemma:

Let $(x^{(1)}, x^{(2)}, \dots, x^{(t)}, \dots)$ denote the sequence of permutations generated by the (1+1)-EA. Let α be an indicator variable defined on permutations of $[n]$ as

$$\alpha(x) = \begin{cases} 1 & x \text{ contains intersections;} \\ 0 & \text{otherwise.} \end{cases}$$

Then $E(\sum_{t=1}^{\infty} \alpha(x^{(t)})) = O\left(n^3 \left(\frac{d_{max}}{d_{min}} - 1\right) \left(\frac{\cos(\epsilon)}{1 - \cos(\epsilon)}\right)\right)$.

For an $m \times m$ grid:

For points on an $m \times m$ grid this bound becomes $O(n^3 m^5)$.

Parameterized Result

Lemma:

Suppose V has k inner points and x is an intersection-free tour on V . Then there is a sequence of at most $2k$ inversions that transforms x into an optimal permutation.

Theorem:

Let V be a set of points quantized on an $m \times m$ and k be the number of inner points. Then the expected optimisation time of the (1+1)-EA on V is $O(n^3 m^5) + O(n^{4k} (2k - 1)!)$.

Summary and Conclusions

- Runtime analysis of RSHs in combinatorial optimization
 - Starting from toy problems to real problems
 - Insight into working principles using runtime analysis
 - General-purpose algorithms successful for wide range of problems
 - Interesting, general techniques
 - Runtime analysis of new approaches possible
- An exciting research direction.

Thank you!

References

-  F. Neumann and C. Witt (2010):
Bioinspired Computation in Combinatorial Optimization – Algorithms and Their Computational Complexity.
Springer.
-  A. Auger and B. Doerr (2011):
Theory of Randomized Search Heuristics – Foundations and Recent Developments.
World Scientific Publishing
-  F. Neumann and I. Wegener (2007):
Randomized local search, evolutionary algorithms, and the minimum spanning tree problem.
Theoretical Computer Science 378(1):32–40.
-  O. Giel and I. Wegener (2003):
Evolutionary algorithms and the maximum matching problem.
Proc. of STACS '03, LNCS 2607, 415–426, Springer
-  B. Doerr, E. Happ and C. Klein (2012):
Crossover can provably be useful in evolutionary computation.
Theoretical Computer Science 425:17–33.
-  C. Witt (2005):
Worst-case and average-case approximations by simple randomized search heuristics.
Proc. of STACS 2005, LNCS 3404, 44–56, Springer.
-  T. Friedrich, J. He, N. Hebbinghaus, F. Neumann and C. Witt (2010):
Approximating covering problems by randomized search heuristics using multi-objective models.
Evolutionary Computation 18(4):617–633.
-  S. Kratsch and F. Neumann (2009):
Fixed-parameter evolutionary algorithms and the vertex cover problem.
In Proc. of GECCO 2009, 293–300. ACM.
-  A. M. Sutton and F. Neumann (2012):
A parameterized runtime analysis of evolutionary algorithms for the Euclidean traveling salesperson problem.
Proc. of AAAI 2012.

88/88