# Bioinspired computation in combinatorial optimization-Algorithms and their computational complexity 

Neumann, Frank; Witt, Carsten

Published in:
Proceeding of the fifteenth annual conference companion on Genetic and evolutionary computation

## Link to article, DOI:

10.1145/2464576.2466738

Publication date:
2013

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

## Citation (APA):

Neumann, F., \& Witt, C. (2013). Bioinspired computation in combinatorial optimization - Algorithms and their computational complexity. In Proceeding of the fifteenth annual conference companion on Genetic and evolutionary computation (pp. 567-590). Association for Computing Machinery.
https://doi.org/10.1145/2464576.2466738

[^0]Bioinspired Computation in Combinatorial Optimization - Algorithms and Their Computational Complexity

Frank Neumann ${ }^{1}$ Carsten Witt ${ }^{2}$
${ }^{1}$ The University of Adelaide
cs.adelaide.edu.au/~frank
${ }^{2}$ Technical University of Denmark
www.imm.dtu.dk/~cawi

Tutorial at GECCO 2013

Copyright is held by the author/owner(s).
GECCO'13 Companion, July 6-10, 2013, Amsterdam, The Netherlands.
АСМ 978-1-4503-1964-5/13/07.


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 $\xrightarrow{x} \xrightarrow{f(x)}$ 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.

## Theoretically considered RSHs

- ( $1+1$ ) EA
- (1+ 1 ) EA (offspring population)
- $(\mu+1)$ EA (parent population)
- $(\mu+1)$ 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

## $(1+1)$ EA and RLS for maximization problems

```
(1+1) EA
    (1) Choose }\mp@subsup{x}{0}{}\in{0,1\mp@subsup{}}{}{n}\mathrm{ uniformly at random.
    (2) For t:= 0,\ldots,\infty
        (0) Create }y\mathrm{ by flipping each bit of }\mp@subsup{x}{t}{}\mathrm{ indep. with probab. 1/n.
        (2) If f(y)\geqf(\mp@subsup{x}{t}{})\mathrm{ set }\mp@subsup{x}{t+1}{}:=y else }\mp@subsup{x}{t+1}{}:=\mp@subsup{x}{t}{}\mathrm{ .
```

RLS
(1) Choose $x_{0} \in\{0,1\}^{n}$ uniformly at random.
(2) For $t:=0, \ldots, \infty$
(1) Create $y$ by flipping one bit of $x_{t}$ uniformly.
(2) If $f(y) \geq f\left(x_{t}\right)$ set $x_{t+1}:=y$ else $x_{t+1}:=x_{t}$.

- 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


## Early 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.

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
(1) The origins: example functions and toy problems - A simple toy problem: OneMax for $(1+1) \mathrm{EA}$
(2) Combinatorial optimization problems

- Minimum spanning trees
- Maximum matchings
- Shortest paths
- Makespan scheduling
- Covering problems
- Traveling salesman problem
EndReferences

```
Simple example functions (test functions)
    - \(\operatorname{OneMax}\left(x_{1}, \ldots, x_{n}\right)=x_{1}+\cdots+x_{n}\)
    - LeadingOnes \(\left(x_{1}, \ldots, x_{n}\right)=\sum_{i=1}^{n} \prod_{j=1}^{i} x_{j}\)
    - BinVal \(\left(x_{1}, \ldots, x_{n}\right)=\sum_{i=1}^{n} 2^{n-i} x_{i}\)
    - 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 ...

## 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

Example: OneMax

The expected runtime of the RLS, $(1+1) E A,(\mu+1) E A,(1+\lambda) E A$ 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\operatorname{log}n).
```

Holds also for population-based ( $\mu+1$ ) EA and for $(1+\lambda)$ EA with small populations.

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

## Later Results Using Toy Problems

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

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

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

$$
\sum_{i=0}^{n-1} \frac{e n}{n-i}=O(n \log n)
$$

- 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
- ...


## Agenda

- 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
(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

Minimum Spanning Trees:

- Given: Undirected connected graph G = (V, E) with $n$ vertices and $m$ edges with positive integer weights.
- Find: Edge set $\mathrm{E}^{\prime} \subseteq \mathrm{E}$ with minimal weight connecting all vertices.
- Search space $\{0,1\}^{m}$
- Edge $e_{i}$ is chosen iff $x_{i}=1$
- Consider (1+1) EA


## 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.

First goal: Obtain a connected subgraph of G.

How long does it take?

Connected graph in expected time $\mathrm{O}(\mathrm{mlog} \mathrm{n})$
(fitness-based partitions)

Bijection for minimum spanning trees:


## Upper Bound

Theorem:
The expected time until (1+1) EA constructs a
minimum spanning tree is bounded by $0\left(\mathrm{~m}^{2}(\log \mathrm{n}+\right.$ $\left.\log w_{\max }\right)$ ).

Sketch of proof:

- w(s) weight current solution s.
- $w_{\text {opt }}$ weight minimum spanning tree $T^{*}$
- set of $m+1$ operations to reach $T^{*}$
- $m^{\prime}=m-(n-1) 1$-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 $\left(w(s)-w_{\text {opt }}\right) /(m+1)$


## 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 $1-(1 /(2 n))$
- Probability $\left(\mathrm{n} / \mathrm{m}^{2}\right)$ for a good 2-bit flip
- Expected time until q 2-steps $\mathrm{O}\left(\mathrm{qm}^{2} / \mathrm{n}\right)$

Consider 1-steps:

- Expected weight decrease by a factor $1-\left(1 /\left(2 m^{\prime}\right)\right)$
- Probability ( $\mathrm{m}^{\prime} / \mathrm{m}$ ) for a good 1-bit flip
- Expected time until q 1-steps O(qm/m')

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

## Expected Multiplicative Distance <br> Decrease (aka Drift Analysis)



Maximum distance: $\mathrm{w}(\mathrm{s})-\mathrm{w}_{\mathrm{opt}} \leq \mathrm{D}:=\mathrm{m} \cdot \mathrm{wmax}$
1 step: Expected distance at most (1-1/(2n))(w(s) $\mathrm{w}_{\mathrm{opt}}$ )
$t$ steps: Expected distance at most $(1-1 /(2 n))^{t}(w(s)-$ $\mathrm{w}_{\text {opt }}$ )
$t:=\lceil 2 \cdot(\ln 2) n(\log D+1)\rceil:(1-1 /(2 n))^{t}\left(w(s)-w_{\text {opt }}\right) \leq 1 / 2$
Expected number of 2 -steps $2 \mathrm{t}=\mathrm{O}\left(\mathrm{n}\left(\log \mathrm{n}+\log \mathrm{w}_{\max }\right)\right)($ Markov $)$

Expected optimization time
$\mathrm{O}\left(\mathrm{tm}^{2} / \mathrm{n}\right)=\mathrm{O}\left(\mathrm{m}^{2}\left(\log \mathrm{n}+\log \mathrm{w}_{\max }\right)\right)$.

## Maximum Matchings

(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

Example: whole graph is augmenting path
Interesting: how simple EAs find augmenting paths

## 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

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

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 $O\left(n^{4}\right)$.

## Maximum Matchings: Upper Bound (Ctnd.)

Proof idea for $O\left(n^{4}\right)$ bound

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

- Length changes according to a fair random walk $\rightarrow$ equal probability for lengthenings and shortenings


## 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 $\{0, \ldots, n\}$ takes in expectation $O\left(n^{2}\right)$ steps.

## Maximum Matchings: Upper Bound (Ctnd.)

Proof idea for $O\left(n^{4}\right)$ bound

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


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


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).

## Maximum Matching: Approximations

## Agenda

Insight: do not hope for exact solutions but for approximations
For maximization problems: solution with value $a$ is called $(1+\varepsilon)$-approximation if $\frac{\mathrm{OPT}}{a} \leq 1+\varepsilon$, where OPT optimal value.

## Theorem <br> For $\varepsilon>0$, $(1+1)$ EA finds a $(1+\varepsilon)$-approximation of a maximum matching in expected time $O\left(\mathrm{~m}^{2 / \varepsilon+2}\right)$ ( $m$ 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.
(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
(4) References


## All-pairs-shortest-path (APSP) problem

Given: Connected directed graph $G=(V, E),|V|=n$ and $|E|=m$, and a function $w: E \rightarrow N$ 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 $v_{j} \in V \backslash\left\{v_{i}\right\}$

## Representation:

Individuals are paths between two particular vertices $v_{i}$ and $v_{j}$

Initial Population:

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

## Mutation-based EA

## Mutation:

Pick individual $\mathrm{I}_{\mathrm{u}, \mathrm{v}}$ uniformly at random


Pick uniformly at random an edge $e=(x, y) \in E^{-}(u) \cup E^{+}(v)$
Add e
New individual $l_{\mathrm{s}, \mathrm{t}}$

## Steady State EA

1. Set $P=\left\{I_{u, v}=(u, v) \mid(u, v) \in E\right\}$.
2. Choose an individual $I_{x, y} \in P$ uniformly at random.
3. Mutate $I_{x, y}$ to obtain an individual $I_{s, t}^{\prime}$.
4. If there is no individual $I_{s, t} \in P, P=P \cup\left\{I_{s, t}^{\prime}\right\}$, else if $f\left(I_{s, t}^{\prime}\right) \leq f\left(I_{s, t}\right), P=\left(P \cup\left\{I_{s, t}^{\prime}\right\}\right) \backslash\left\{I_{s, t}\right\}$
5. Repeat Steps $2-4$ forever.

## Lemma:

Let $\ell \geq \log n$. The expected time until has found all shortest paths
with at most $\ell$ edges is $O\left(n^{3} \ell\right)$.
Proof idea:
Consider two vertices $u$ and $v, u \neq v$.
Let $\gamma:=\left(v^{1}=u, v^{2}, \ldots, v^{\ell^{\prime}+1}=v\right)$ be a shortest path
from $u$ to $v$ consisting of $\ell^{\prime}, \ell^{\prime} \leq \ell$, edges in $G$
the sub-path $\gamma^{\prime}=\left(v^{1}=u, v^{2}, \ldots, v^{j}\right)$ is a shortest path from $u$ to $v^{j}$.


Population size is upper bounded $\mathrm{n}^{2}$ (for each pair of vertices at most one path)

- Pick shortest path from $u$ to $v_{j}$ and append edge ( $\mathrm{v}_{\mathrm{j}}, \mathrm{v}_{\mathrm{j}+1}$ )
- 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 $1 /(2 n)$
- Success with probability at least $p=1 /\left(2 n^{3}\right)$
- At most I successes needed to obtain shortest path from $u$ to $v$


## Analysis

Consider typical run consisting of $\mathrm{T}=\mathrm{cn}^{3} \mid$ steps.
What is the probability that the shortest path from $u$ to $v$ has been obtained?
We need at most I successes, where a success happens in each step with probability at least $p=1 /\left(2 n^{3}\right)$

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

$$
\operatorname{Prob}\left(X_{i}=1\right) \geq p=1 /\left(2 n^{3}\right) \quad X=\sum_{i=1}^{T} X_{i} \quad X \geq \ell ? ? ?
$$

Expected number of successes $E(X) \geq T /\left(2 n^{3}\right)=\frac{c n^{3} \ell}{2 n^{3}}=\frac{c \ell}{2}$
Chernoff: $\quad \operatorname{Prob}(X<(1-\delta) E(x)) \leq e^{-E(X) \delta^{2} / 2}$
$\delta=\frac{1}{2}$
$\operatorname{Prob}\left(X<\left(1-\frac{1}{2}\right) E(x)\right) \leq e^{-E(X) / 8} \leq e^{-T /\left(16 n^{3}\right)}=e^{-c n^{3} \ell /\left(16 n^{3}\right)}=e^{-c \ell /(16)}$
Probability for failure of at least one pair of vertices at most: $n^{2} \cdot e^{-c \ell / 16}$
$c$ large enough and $\ell \geq \log n$ :
No failure in any path with probability at least $\alpha=1-n^{2} \cdot e^{-c \ell / 16}=1-o(1)$
Holds for any phase of T steps
Expected time upper bound by $T / \alpha=O\left(n^{3} \ell\right)$

Shortest paths have length at most $\mathrm{n}-1$.
Set $\mathrm{I}=\mathrm{n}-1$

Theorem
The expected optimization time of Steady State EA for the APSP problem is $O\left(n^{4}\right)$.

## Remark:

There are instances where the expected optimization of $(\mu+1)$-EA is $\Omega\left(n^{4}\right)$
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 $P=\left\{I_{u, v}=(u, v) \mid(u, v) \in E\right\}$.
2. Choose $r \in[0,1]$ uniformly at random.
3. If $r \leq p_{c}$, choose two individuals $I_{x, y} \in P$ and $I_{x^{\prime}, y^{\prime}} \in P$ uniformly at random and perform crossover to obtain an individual $I_{s, t}^{\prime}$,
else choose an individual $I_{x, y} \in P$ uniformly at random and mutate $I_{x, y}$ to obtain an individual $I_{s, t}^{\prime}$.
4. If $I_{s, t}^{\prime}$ is a path from $s$ to $t$ then

丸 If there is no individual $I_{s, t} \in P, P=P \cup\left\{I_{s, t}^{\prime}\right\}$,
$\star$ else if $f\left(I_{s, t}^{\prime}\right) \leq f\left(I_{s, t}\right), P=\left(P \cup\left\{I_{s, t}^{\prime}\right\}\right) \backslash\left\{I_{s, t}\right\}$.
5. Repeat Steps 2-4 forever.

## Theorem:

The expected optimization time of Steady State GA is $O\left(n^{3.5} \sqrt{\log n}\right)$.
Mutation and $\ell^{*}:=\sqrt{n \log n}$
All shortest path of length at most $\|^{*}$ 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 I* edges have already been obtained.

Assume that all shortest paths of length $\mathrm{k} \leq I^{*}$
have been obtained.
What is the expected time to obtain all shortest paths of length at most $3 \mathrm{k} / 2$ ?

## Analysis Crossover

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

There are 2 k -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 $2 k+1-r$ possible pairs: probability at least $\left.(2 k+1-r) / n^{4}\right) \geq k /\left(2 n^{4}\right)$

At most $n^{2}$ shortest paths of length $r, k<r \leq 3 k / 2$
Time to collect all paths $\mathrm{O}\left(\mathrm{n}^{4} \log \mathrm{n} / \mathrm{k}\right)$
(similar to Coupon Collectors Theorem)

## Analysis Crossover

Sum up over the different values of $k$, namely

$$
\sqrt{n \log n}, c \cdot \sqrt{n \log n}, c^{2} \cdot \sqrt{n \log n}, \ldots, c^{\log _{c}(n / \sqrt{n \log n})} \cdot \sqrt{n \log n}
$$

where $c=3 / 2$.

Expected Optimization
$\sum_{s=0}^{\log _{c}(n / \sqrt{n \log n})}\left(O\left(\frac{n^{4} \log n}{\sqrt{n \log n}}\right) c^{-s}\right)=O\left(n^{3.5} \sqrt{\log n}\right) \sum_{s=0}^{\infty} c^{-s}=O\left(n^{3.5} \sqrt{\log n}\right)$
(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 path
- Makespan scheduling
- Covering problems
- Traveling salesman problem
4 References


## Makespan Scheduling

What about NP-hard problems? $\rightarrow$ Study approximation quality
Makespan scheduling on 2 machines:

- $n$ objects with weights/processing times $w_{1}, \ldots, w_{n}$
- 2 machines (bins)
- Minimize the total weight of fuller bin = makespan.

Formally, find $I \subseteq\{1, \ldots, n\}$ 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

- Problem encoding: bit string $x_{1}, \ldots, x_{n}$ reserves a bit for each object, put object $i$ in bin $x_{i}+1$.
- Fitness function

$$
f\left(x_{1}, \ldots, x_{n}\right):=\max \left\{\sum_{i=1}^{n} w_{i} x_{i}, \sum_{i=1}^{n} w_{i}\left(1-x_{i}\right)\right\}
$$

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


## Sufficient Conditions for Progress

Abbreviate $S:=w_{1}+\cdots+w_{n} \Rightarrow$ 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 $(1+1) E A$ and RLS reach $f$-value $\leq \frac{S}{2}+\frac{s^{*}}{2}$ in expected $O\left(n^{2}\right)$ steps.

## Sufficient Conditions for Progress

Abbreviate $S:=w_{1}+\cdots+w_{n} \Rightarrow$ 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 $O\left(n^{2}\right)$ steps.

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 $O\left(n^{2}\right)$ steps.

## Sufficient Conditions for Progress

Abbreviate $S:=w_{1}+\cdots+w_{n} \Rightarrow$ 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 $R L S$ reach $f$-value $\leq \frac{S}{2}+\frac{s^{*}}{2}$ in expected $O\left(n^{2}\right)$ steps.

## Sufficient Conditions for Progress

Abbreviate $S:=w_{1}+\cdots+w_{n} \Rightarrow$ 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 $(1+1) E A$ and $R L S$ reach $f$-value $\leq \frac{S}{2}+\frac{s^{*}}{2}$ in expected $O\left(n^{2}\right)$ steps.

## Worst-Case Results

## Theorem

On any instance to the makespan scheduling problem, the $(1+1) E A$ and $R L S$ reach a solution with approximation ratio $\frac{4}{3}$ in expected time $O\left(n^{2}\right)$.

Use study of object sizes and previous lemma.

## Theorem

There is an instance $W_{\varepsilon}^{*}$ 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 $4 / 3-\varepsilon$.

## Sufficient Conditions for Progress

Abbreviate $S:=w_{1}+\cdots+w_{n} \Rightarrow$ 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 $(1+1) E A$ and RLS reach $f$-value $\leq \frac{S}{2}+\frac{s^{*}}{2}$ in expected $O\left(n^{2}\right)$ steps.

## Worst-Case Instance

Instance $W_{\varepsilon}^{*}=\left\{w_{1}, \ldots, w_{n}\right\}$ is defined by $w_{1}:=w_{2}:=\frac{1}{3}-\frac{\varepsilon}{4}$ (big objects) and $w_{i}:=\frac{1 / 3+\varepsilon / 2}{n-2}$ for $3 \leq i \leq n, \varepsilon$ 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 $\frac{2}{3}-\frac{\varepsilon}{2}$.
Move a big object in the emptier bin $\Rightarrow$ value $\left(\frac{1}{3}+\frac{\varepsilon}{2}\right)+\left(\frac{1}{3}-\frac{\varepsilon}{4}\right)=\frac{2}{3}+\frac{\varepsilon}{4}!$
Need to move $\geq \varepsilon n$ small objects at once for improvement: very unlikely.


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

## Worst Case - PRAS by Parallelism

## Worst Case - PRAS by Parallelism (Proof Idea)

Set $s:=\left\lceil\frac{2}{\varepsilon}\right\rceil$
Assuming $w_{1} \geq \cdots \geq w_{n}$, we have $w_{i} \leq \varepsilon \frac{S}{2}$ for $i \geq s$.

## Theorem

On any instance, the $(1+1)$ EA and RLS with prob. $\geq 2^{-c \mid 1 / \varepsilon\rceil \ln (1 / \varepsilon)}$ 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)!

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.

## Average-Case Analyses

Models: each weight drawn independently at random, namely
(c) uniformly from the interval $[0,1]$,
(- exponentially distributed with parameter 1 (i.e., $\operatorname{Prob}(X \geq t)=e^{-t}$ 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?

```
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?
```


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

## Theorem

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

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 $>2\left(X_{(i)}-X_{(i+1)}\right)>0$, then objects can be swapped; discrepancy falls Consider such "difference objects".

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


## A Parameterized Analysis

Have seen: problem is hard for $(1+1) \mathrm{EA} / \mathrm{RLS}$ 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 $f(k) \cdot$ 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
( Unbalance of optimal solution

## Value of Optimal Solution

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

Since $w_{1} \geq \cdots \geq w_{n}$, 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
$(1+1) E A$ and RLS find solution of makespan $\leq S / 2+S / k$ with probability $\Omega\left((2 k)^{-e k}\right)$ in time $O(n \log k)$. Multistarts have success probability $\geq 1 / 2$ after $O\left(2^{(e+1) k} k^{e k} n \log k\right)$ evaluations.
$2^{(e+1) k} k^{e k} \log k$ does not depend on $n \rightarrow$ a randomized FPT-algorithm.

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 <br> For critical path size $k$, multistart RLS finds optimum in $O\left(2^{k}(e n)^{c k} n \log n\right)$ evaluations with probability $\geq 1 / 2$.

Due to term $n^{c k}$, 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.

## Unbalance of Optimal Solution

Consider discrepancy of optimum $\Delta^{*}:=2(\mathrm{OPT}-S / 2)$.
Question/decision problem: Is $w_{k} \geq \Delta^{*} \geq w_{k+1}$ ?
Observation: If $\Delta^{*} \geq w_{k+1}$, optimal solution will put $w_{k+1}, \ldots, w_{n}$ on emptier machine. Crucial to distribute first $k$ objects optimally.

## Theorem

Multistart RLS with biased mutation (touches objects $w_{1}, \ldots, w_{k}$ with prob. $1 /(k n)$ each $)$ solves decision problem in $O\left(2^{k} n^{3} \log n\right)$ evaluations with probability $\geq 1 / 2$.

Again, a randomized FPT-algorithm.
(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
(4) References


## 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!!!

The Problem
Integer Linear Program (ILP)
$\min \sum_{i=1}^{n} x_{i}$$\quad \forall\{i, j\} \in E$

Decision problem: Is there a set of vertices of size at most k covering all edges?
Our parameter: Value of an optimal solution (OPT)

## Evolutionary Algorithm

Representation: Bitstrings of length n
Minimize fitness function:

$U(x)$ : Edges not covered by $x$
$G(x)=G(V, U(x))$
$L P(x)$ : value of LP applied to $G(x)$

## Evolutionary Algorithm



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

Multi-Objective Approach:
Treat the different objectives in the same way



## What can we say about these solutions?


${ }^{|x|_{1}} \boldsymbol{\Delta}$

Q
Q. $\quad$.


## 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 $L P(x)=L P\left(0^{n}\right)-|x|_{1}$ are Pareto optimal.
They can be extended to minimum vertex cover by selecting additional vertices.

## Approximations



## Euclidean TSP

(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

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.

## Representation and Mutation

Representation: Permutation of the n cities

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

Inversion (inv) as mutation operator:

- Select $\mathrm{i}, \mathrm{j}$ from $\{1, \ldots \mathrm{n}\}$ 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)


## (1+1) EA

$x \leftarrow$ a random permutation of $[n]$.
repeat forever
$y \leftarrow \operatorname{Mutate}(x)$
if $f(y)<f(x)$ then $x \leftarrow y$
Mutation:
(1+1) EA: k random inversion, $k$ chosen according to
1+Pois(1)

## Intersection and Mutation



Convex hull containing $n-k$ points


## 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 $\theta$ 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 $\varepsilon$

## Progress

## Assumptions:

$\mathrm{d}_{\text {max }}$ : Maximum distance between any two points
$d_{\text {min }}$ : Minimum distance between any two points
$V$ is angle-bounded by $\varepsilon$
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, $f(x)-f(y)>2 d_{\text {min }}\left(\frac{1-\cos (\epsilon)}{\cos (\epsilon)}\right)$.

## Tours

A tour x is either

- Intersection free
- Non intersection free

Intersection free tour 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 $\left(x^{(1)}, x^{(2)}, \ldots, x^{(t)}, \ldots\right)$ denote the sequence of permutations generated by the ( $1+1$ )-EA. Let $\alpha$ 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 $E\left(\sum_{t=1}^{\infty} \alpha\left(x^{(t)}\right)\right)=O\left(n^{3}\left(\frac{d_{\max }}{d_{\text {min }}}-1\right)\left(\frac{\cos (\epsilon)}{1-\cos (\epsilon)}\right)\right)$.

For an m x m grid:
For points on an $m \times m$ grid this bound becomes $O\left(n^{3} m^{5}\right)$.

## Summary and Conclusions

## 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 $2 k$ 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 $O\left(n^{3} m^{5}\right)+O\left(n^{4 k}(2 k-1)!\right)$.

- 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
$\rightarrow$ An exciting research direction.


## References

 Bioinspired Computation in Combinatorial Optimization - Algorithms and Their Computational Complexity
A. Auger and B. Doerr (2011)

Theory of Randomized Search Heuristics - Foundations and Recent Developments,
冨
Randomized local search, evolutionary algorithms, and the minimum spanning tree problem
風 O. Giel and I. Wegener (2003): Evolutionary algorithms and the maximum matching problem.
Proc. of STACS ' 03 , LNCS 2607 415-426. Sp
B. Doerr, E. Happ and C. Klein (2012): Crossover can provably be useful in evolutionary computation.
( E - Witt (2005): Wrorst-ase and averacs 2 -case approximations by simple randomized search heuristics
T. Friedrich

Approximating covering problems by randomized search heuristics using multi-objective models.
S. Kratsch and F. Neumann (2009) Fixed-parameter evolutionary algorithms and the vertex cover problem.
A. M. Sutton and F. Neumann (2012): A parameterized runtime analysis of evolutionary algorithms for the Euclidean traveling salesperson problem.


[^0]:    General rights
    Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

    - Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
    - You may not further distribute the material or use it for any profit-making activity or commercial gain
    - You may freely distribute the URL identifying the publication in the public portal

