

Theory of estimation-of-distribution algorithms

Witt, Carsten

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Theory of Estimation-of-Distribution Algorithms

Carsten Witt

DTU Compute Technical University of Denmark

Tutorial at GECCO 2019 Updated version: https://tinyurl.com/eda2019

GECCO '19 Companion, July 13–17, 2019, Prague, Czech Republic. © 2019 Copyright is held by the author/owner(s). ACM ISBN 978-1-4503-6748-6/19/07. https://doi.org/10.1145/3319619.3323367

Theory of EDAs > Introduction

INSTRUCTOR

Carsten Witt is an associate professor at the Technical University of Denmark. He received his M. Sc. in 2000 and Ph. D. degree in 2004, both in Computer Science from the Technical University of Dortmund, Germany. His main expertise is in the algorithmic analysis of metaheuristics, including evolutionary algorithms, ant colony optimization and estimation-of-distribution algorithms. Carsten has over 80 peer-reviewed publications and has given tutorials about bio-inspired computation in combinatorial optimization at previous GECCO and PPSN conferences. He is member of the editorial boards of Evolutionary Computation Journal and Theoretical Computer Science.



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EVOLUTIONARY VS. ESTIMATION-OF-DISTRIBUTION ALGORITHMS

Evolutionary Algorithms (EAs)

- Work with populations of search points
- Modify the search points through, e. g., mutation and crossover
- Select promising search points based on fitness

EDAs

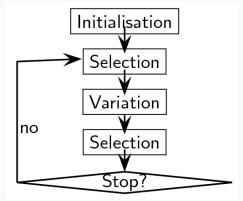
- Work with probability distributions
- Sample search points based on current distribution
- Adjust distribution based on the most promising search points

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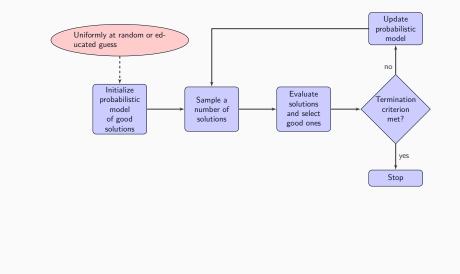
OVERVIEW

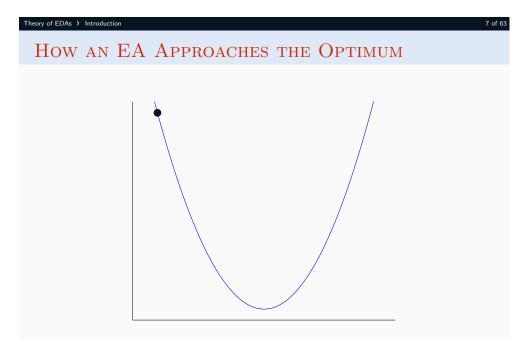
- Introduction to estimation-of-distribution algorithms (EDAs)
- ► What do we mean by theory?
- Presentation of important EDAs in theory
- Main results: from convergence to runtime analysis
- Conclusions

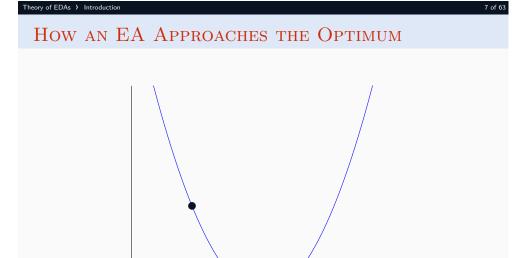
A CLASSICAL EVOLUTIONARY ALGORITHM



AN ESTIMATION-OF-DISTRIBUTION ALGORITHM

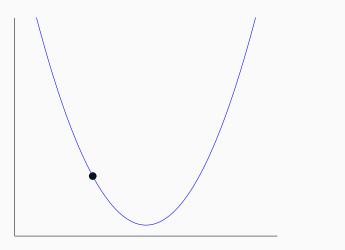






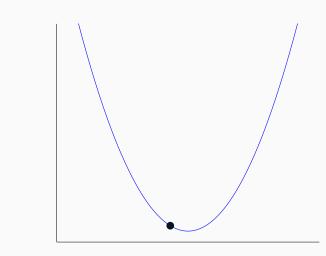
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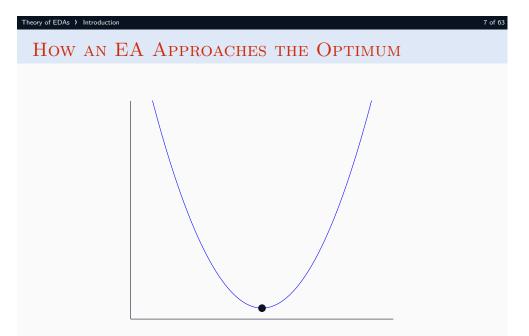
HOW AN EA APPROACHES THE OPTIMUM



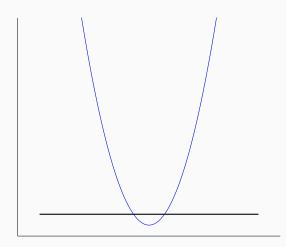
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HOW AN EA APPROACHES THE OPTIMUM

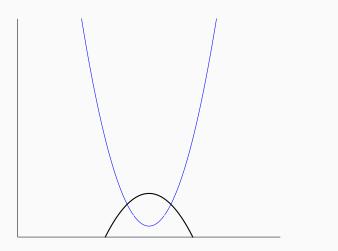








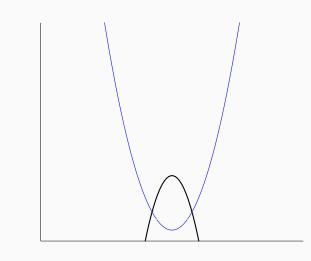
How an EDA Adjusts the Probabilistic Model



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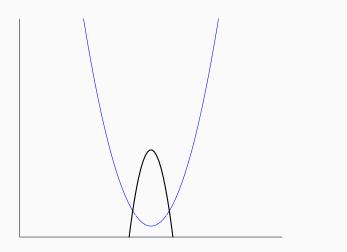
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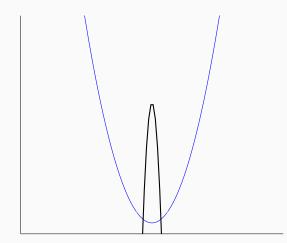
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How an EDA Adjusts the Probabilistic Model



Theory of EDAs > Introduction





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Preliminaries

OneMax

LeadingOnes

BinaryValue

Noise

Jump

Stable EDAs

End

heory of EDAs) Preliminaries

IMPORTANT EDAS

Domain: discrete optimization, e.g., find maximum for $f : \{0, 1\}^n \to \mathbb{R}$. Important distinction: univariate vs. multivariate EDAs.

For example: $f(x_1, x_2, x_3) = -x_1 + 2x_1x_2 + x_3$. Good to learn learn dependency between x_1 and x_2 .

Univariate

▶ ...

- ► cGA
- ► UMDA
- PBIL
- MMAS

Multivariate ► FDA

- ECGA
- MIMIC, BMDA
- BOA

Most theoretical results concern univariate EDAs.

Theory of EDAs) Preliminaries

Some Benchmark Functions

Theoretical results often consider simple problems, which we have to understand first.

• ONEMAX $(x_1, \ldots, x_n) := \sum_{i=1}^n x_i$



- BINVAL $(x_1, ..., x_n) := \sum_{i=1}^n 2^{n-i} x_i$
- LEADINGONES $(x_1, \ldots, x_n) := \sum_{i=1}^n \prod_{i=1}^i x_i$

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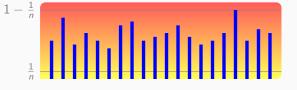
Illustrate simple but fundamental properties; re-appear in more complex scenarios.

Write ONEMAX but mean n - Ham(x, a) for unknown string $a \in \{0, 1\}^n$.

Theory of EDAs) Preliminaries

UNIVARIATE ALGORITHMS

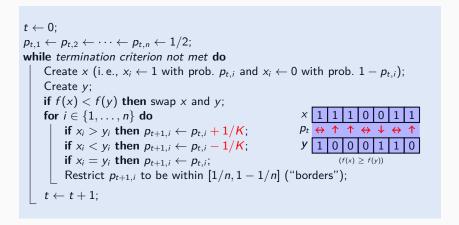
Common concept: the frequency vector (aka. marginal probabilities)



- Probabilities (p_1, \ldots, p_n) for setting the individual bits to 1.
- Usually initialized as $p_i = 1/2$ for all *i*.
- Independently sampled.
- ► Frequency vector adjusted over time.

Compact GA (cGA) (Harik et al., 1999)

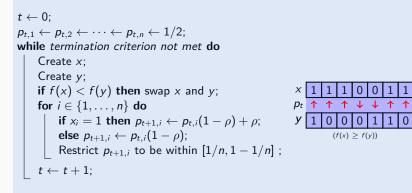
Simulates behavior of a GA with population size K in a compact way.



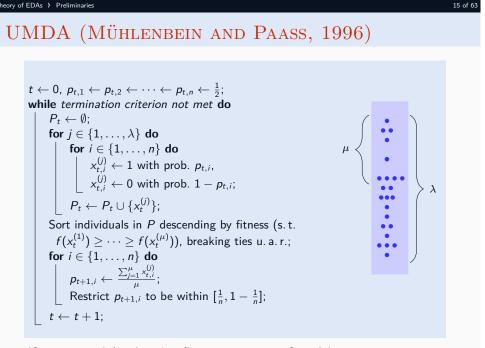
Parameter K determines preciseness of model. Big K = fine model = small update strength.

2-MMAS_{IB} (Neumann et al., 2010)

Max-Min Ant System (Stützle and Hoos, 2000) with iteration-best update



Here $1/\rho$ reflects preciseness.



Theory of EDAs) Preliminaries

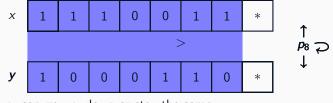
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Adjustment of frequencies: a general challenge

Frequencies may walk into the wrong direction

- ▶ if the fitness function gives wrong hints w.r.t. single bits,
- ▶ if the function gives no hints but algorithm must update,
- even if the fitness function overall gives the right hints.

Think of ONEMAX:



 p_8 can go up, down or stay the same.

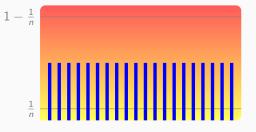
If, e.g., $\mu = \lambda/2$, then λ reflects preciseness of model.

Theory of EDAs) Preliminaries

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GENETIC DRIFT

If the fitness function is constant/flat (does not give a signal), frequencies move randomly to a border (DEMO).

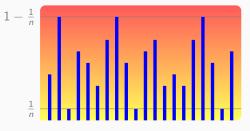


Frequencies that move to the wrong border are problematic – even disastrous if the border is not there.

Even if the expected value of a frequency converges to optimal value (Höhfeld and Rudolph, 1997), this does not say much about runtime.

GENETIC DRIFT

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Contents		Early Results (< 2000)
Introduction		Models of cGA, UMDA and others, allowing estimations of the dynamical behavior (e.g., Thierens et al., 1998; Mühlenbein and Mahnig, 1999). Two effects:
Preliminaries OneMax		1. Overall progress of probabilistic model (roughly: $\sum p_i$) and time to convergence to good distribution ($\sum p_i \approx n$),
LeadingOnes		2. time for single frequencies to drift to wrong border by genetic drift \rightarrow should be bigger than convergence time.
BinaryValue		Avoiding genetic drift requires precise enough model \rightarrow lower bound on runtime. Models of EDAs estimated progress of frequencies:
Noise		Mühlenbein and Mahnig (1999)
Jump		Wunienbein and Wannig (1999)
Stable EDAs		$p_{t+1,i}pprox p_{t,i} + rac{l}{\sqrt{n}} \sqrt{p_{t,i} \Big(1-p_{t,i}\Big)} \; ,$
End		
		which was made rigorous recently.

FIRST STEPS TOWARDS RUNTIME ANALYSES

Genetic drift recurrent issue in analysis of GAs and EDAs, e.g., Asoh and Mühlenbein (1994); Shapiro (2003, 2005). Models proposed to make frequencies "stable" (Friedrich et al., 2016a) \rightarrow later.

Lower bound on preciseness of model

For different EDAs on ONEMAX, same threshold identified multiple times (Thierens et al., 1998; Lobo et al., 2000; Shapiro, 2005): need at least $K = \Omega(\sqrt{n})$ different frequency values to prevent genetic drift.

Upper bound on time to convergence

Time for the EDA to converge to optimal solution $\approx K\sqrt{n}$.

 \Rightarrow Best possible time complexity $\Theta(n)$?

heory of EDAs) OneMax

Pros

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RIGOROUS VS. NON-RIGOROUS ANALYSES

All (?) analyses of convergence speed of EDAs before 2005 made some simplifying assumptions.

Cons

- Unimportant details ignored
- Insights possible that rigorous analyses cannot achieve

 No estimation of errors: verification by experiments

No theorem: may only hold for small problem sizes

Since 2005: rigorous runtime analyses of EDAs, following the same principle as runtime analysis of EAs.

heory of EDAs) OneMax

FIRST RUNTIME ANALYSIS OF EDAS

Droste (2006) considered cGA on ONEMAX (and other functions). Studied runtime = no. iterations until optimum found.

Main results

- Upper bound $O(K\sqrt{n})$ on ONEMAX, for $K = \Omega(n^{1/2+\varepsilon})$ \rightarrow runtime $O(n^{1+\varepsilon})$ (with high probability)
- General lower bound $\Omega(K\sqrt{n})$.

Recent refinement: Upper bound $O(n \log n)$ (Sudholt and W., 2016) for $K = c\sqrt{n} \log n$, big constant c

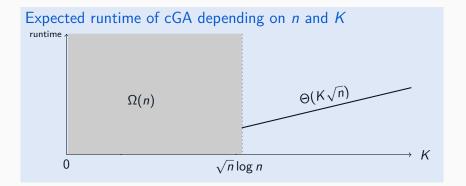
 \Rightarrow competitive with simple EAs (e.g., (1+1) EA).

Best lower bound until 2016: $\Omega(n)$ from general black-box complexity (Doerr and Lengler, 2015)

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Demo and Landscape



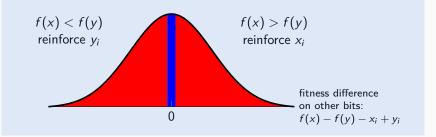
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PROOF IDEA IN THE "LARGE K" REGIME

- Show limits on genetic drift: with high prob. all frequencies stay above 1/3 in a phase of $\Theta(K\sqrt{n})$ steps.
- Frequencies move smoothly upwards (DEMO).
- To analyze speed: consider $\Phi_t = \sum_{i=1}^n p_{t,i}$ and analyze its drift. Important: how does a single frequency evolve?
- Consider the two offspring x and y and look into bit i.

DYNAMICS ON BIT i

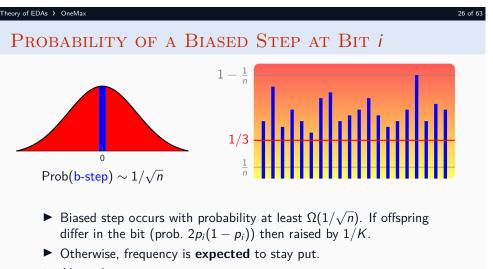
If $x_i = y_i$ then $p_{t,i}$ is unchanged. If $x_i \neq y_i$ then $p_{t,i}$ is changed depending on f(x) vs. f(y):



Red area: bit *i* is irrelevant in this step \Rightarrow genetic drift moves $p_{t,i}$ in a random direction $\pm 1/K$ (rw-step)

Blue area: bit *i* decides the outcome of f(x) vs. f(y) \Rightarrow increase $p_{t,i}$ (b-step, learning that 1s are better than 0s)

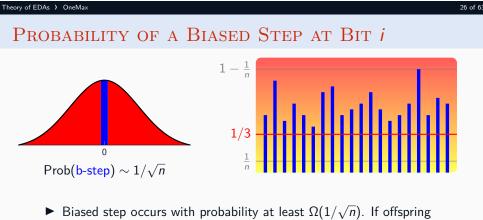
Slide kindly provided by D. Sudholt



Altogether:

 $p_{t+1,i} = p_{t,i} + \Omega(p_{t,i}(1-p_{t,i})/\sqrt{n})$

Note similarity to $p_{t+1,i} \approx p_{t,i} + \frac{I}{\sqrt{n}} \sqrt{p_{t,i} \left(1 - p_{t,i}\right)}$ by Mühlenbein and Mahnig (1999)



- differ in the bit (prob. $2p_i(1-p_i)$) then raised by 1/K.
- Otherwise, frequency is expected to stay put.
- Altogether:

$$p_{t+1,i} = p_{t,i} + \Omega(p_{t,i}(1-p_{t,i})/\sqrt{n})$$

Note similarity to $p_{t+1,i} \approx p_{t,i} + \frac{I}{\sqrt{n}} \sqrt{p_{t,i} \left(1 - p_{t,i}\right)}$ by Mühlenbein and Mahnig (1999)

What Happens for Small K

Now look into $K < \sqrt{n} \log n$:

- Lower bound $\Omega(n)$ until 2015.
- Improved to $\Omega(n \log n)$ (Sudholt and W., 2016).
- Heavy genetic drift occurs.

DEMO.

heory of EDAs) OneMax

Whether optimum can be found at all, depends very much on the borders on the frequencies.

- ► If no borders, with high probability frequencies locked to 0 ⇒ infinite runtime.
- ► If borders {1/n, 1 1/n} used, optimum can still be found in polynomial time! No proof for cGA, but for UMDA (Lehre and Nguyen, 2017; W., 2017).
- \Rightarrow Borders may make the algorithm efficient despite genetic drift.

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IDEA FOR THE LOWER BOUND

Coupon collector

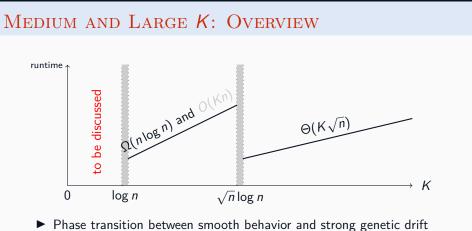
You have to collect *n* different coupons. In each round, you are given one coupon chosen uniformly at random with replacement. In expectation, it takes $\Omega(n \log n)$ rounds to collect all of them.



CC-BY-SA-4.0 by Jarek Tuszyński, 2015

Here the coupons are the frequencies at the lower border. Each of them has probability 1/n of being raised.

If many frequencies move to the lower border before optimum is found, we cannot be faster than $n \log n$.



- ▶ Phase transition between smooth behavior and strong genetic drift at $K \sim \sqrt{n} \log n$
- If no borders, algorithm fails at $K = o(\sqrt{n} \log n)$
- With borders, efficient behavior as long as K = ω(log n).
 Upper bound O(Kn) only conjectured here.

SMALL K

Theory of EDAs) OneMax

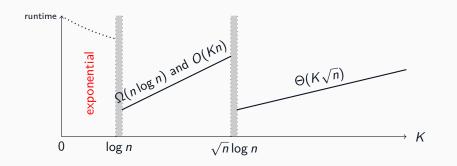
What happens if $K = o(\log n)$? Known for 2-MMAS_{ib} (Neumann et al., 2010), similar to cGA: landslides of frequencies occur.

DEMO.

Frequency that have attained their maximum 1 - 1/n are nevertheless likely to drop down to minimum.

Very unstable behavior, exponential optimization time.

RUNTIME OF CGA ON ONEMAX: COMPLETE PICTURE



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ANALYSIS OF UMDA

How does UMDA perform on ONEMAX?

Surprisingly, in terms of runtimes (no. of iterations $\cdot \lambda$), not very differently from cGA.

Obstacles in analysis:

- frequencies can change drastically, even from minimum to maximum in one generation,
- two parameters: μ and λ .

The first runtime analysis of UMDA on ONEMAX stems from 2015!

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RESULTS FOR UMDA: UPPER BOUNDS

First runtime result (Dang and Lehre, 2015): expected runtime of UMDA on ONEMAX is $O(n\lambda \log \lambda)$ for $\lambda > 13e\mu$ and $\lambda = \Omega(\log n)$. Bound is $O(n \log n \log \log n)$ for best possible parameter setting.

Bound independently improved to $O(n \log n)$ by Lehre and Nguyen (2017) and W. (2017):

Theorem (Expected runtime of UMDA on ONEMAX)

- 1. For constant a > 0 and constant $c \in (0, 1)$, assume $a \ln n \le \mu \le \sqrt{n(1-c)}$, $\lambda \ge (13e)\mu/(1-c) \Rightarrow$ runtime $O(\lambda n)$.
- 2. Assume $\lambda = (1 + \beta)\mu$ for constant $\beta > 0$, $\mu \ge c \log n$ for large constant c > 0, as well as $\mu = o(n) \Rightarrow$ runtime $O(\lambda n)$.
- 3. Assume $\lambda = (1 + \beta)\mu$ for constant $\beta > 0$, $\mu \ge c\sqrt{n}\log n$ for large constant $c > 0 \Rightarrow$ runtime $O(\lambda\sqrt{n})$.

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RESULTS FOR UMDA: LOWER BOUNDS

We also obtain similar bounds as with cGA:

Theorem (Krejca and W., 2017)

Let $\lambda = (1 + \beta)\mu$ for some constant $\beta > 0$ and $\lambda = n^{O(1)}$. Then the expected optimization time of UMDA on ONEMAX is $\Omega(\lambda\sqrt{n} + n \log n)$.

Proof idea again: at a very high level, we estimate

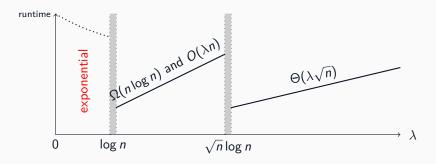
1. progress (drift) of sum of frequencies per iteration

2. time for genetic drift to move frequencies to wrong border both for upper and lower bounds. Especially 2. is challenging.

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Overview of Runtime Bound for UMDA on OneMax



- Exponential time below log *n* strongly conjectured.
- ► Remaining bounds proved.
- If no borders on frequencies, runtime infinite below $\sqrt{n} \log n$

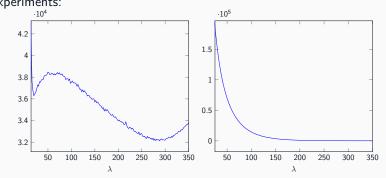
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WHAT HAPPENS IN THE MEDIUM REGIME

If $\lambda = \omega(\log n)$ and $\lambda = o(\sqrt{n})$

 \Rightarrow expected runtime $O(\lambda n)$ and $\Omega(n \log n)$.

Take, e.g., $\lambda = n^{1/3} \Rightarrow$ upper bound $O(n^{4/3})$, lower bound $\Omega(n \log n)$. Again upper bound $O(n \log n)$ for $\lambda = c\sqrt{n} \log n$. Where is the truth? Experiments:



Left: average runtime; right: no. times frequency hits minimum. In fact a multimodal behavior: is $O(\lambda n)$ also $\Omega(\lambda n)$ in medium regime?

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NEW RESULT: RUNTIME OF CGA IS MULTIMODAL

The multimodal behavior has been made rigorous for the simpler cGA, not yet for UMDA.

Theorem (Lengler et al., 2018)

Expected runtime of cGA on ONEMAX is $\Omega(K^{1/3}n + n \log n)$ for $K = O(\sqrt{n}/\log^2 n)$.

⇒ Setting $K = \Theta(\log n)$ gives us runtime $\Theta(n \log n)$, so does $K = \Theta(\sqrt{n} \log n)$, but values in between make runtime worse.

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ONEMAX: SUMMARY

- ► Simple univariate EDAs like UMDA and cGA (and 2-MMAS_{ib}) have similar runtime behavior on ONEMAX.
- Very sensitive to settings of parameters.
- Two phase transitions.
- Multimodal behavior.
- ► If no borders are used, model must have model of preciseness $\Omega(\sqrt{n} \log n)$ to prevent genetic drift.

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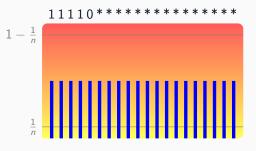
Theory of EDAs) LeadingOnes

EDAS ON LEADINGONES

LEADINGONES(x) = $\sum_{i=1}^{n} \prod_{j=1}^{i} x_j$ has not been considered much in the theory of EDAs (except for UMDA).

Possible reason: behavior is more obvious than on ${\rm ONEMAX}$ and not very different from classical EAs.

Typical: frequencies are optimized from left to right. (DEMO)



If best-so-far solution has *i* leading ones, then last n - i - 1 frequencies are drifting randomly.

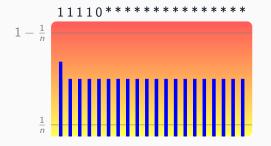
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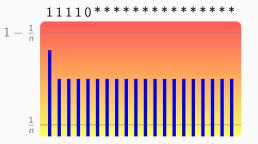
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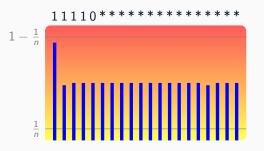
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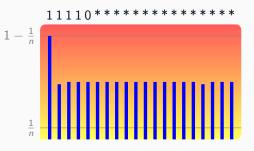
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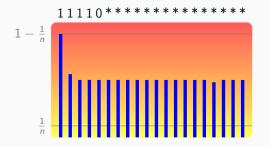
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Theory of EDAs > LeadingOnes

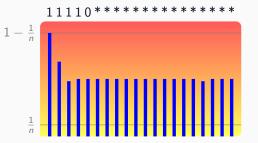
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EDAS ON LEADINGONES

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Possible reason: behavior is more obvious than on ${\rm ONEMAX}$ and not very different from classical EAs.

Typical: frequencies are optimized from left to right. (DEMO)



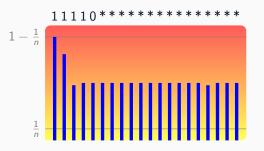
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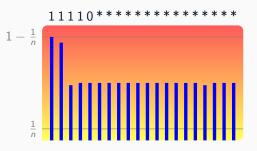
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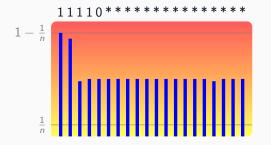
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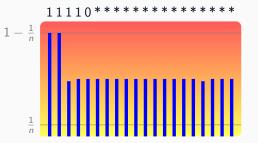
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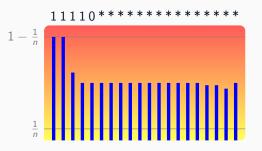
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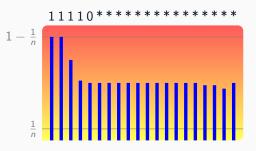
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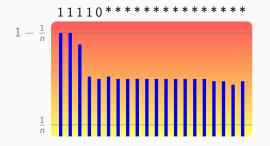
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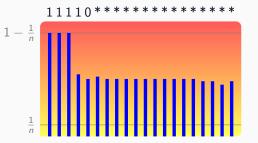
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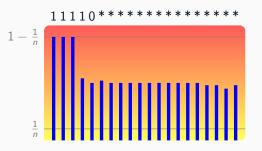
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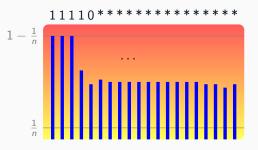
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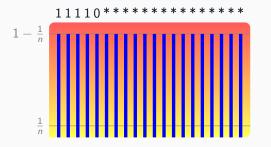
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Theory of EDAs > LeadingOnes

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EARLY RESULTS FOR LEADINGONES

UMDA without borders (Chen et al., 2007, 2009b, 2010):

Using $\lambda = \Omega(n^{2+\varepsilon})$, UMDA (without borders) optimizes LEADINGONES in time $O(\lambda n)$ w. h. p. \Rightarrow runtime $O(n^{3+\varepsilon})$ for optimal λ .

For comparison: (1+1) EA expected runtime $\Theta(n^2)$.

Approach in the analysis again:

- 1. Determine total time for frequency vector to converge to optimality.
- 2. Determine lower bound on preciseness of model to prevent genetic drift before convergence.

Large λ used to prevent genetic drift also for the last optimized bit (possibly too large).

RECENT RESULTS FOR LEADINGONES

WHEN EAS AND EDAS DIFFER ON LEADINGONES

Use the borders.

Theorem (Dang and Lehre, 2015)

If $\lambda \ge c \ln n$ then expected runtime of UMDA with borders on LEADINGONES is $O(n\lambda \log \lambda + n^2)$.

Holds also for PBIL (generalized UMDA) if learning rate not too small (Lehre and Nguyen, 2018).

Overall analysis was similar to ${\rm ONEMAX}.$ No new insights through the study of ${\rm LEADINGONES}?$

Consider following example from Chen et al. (2009a).

heory of EDAs) LeadingOnes

Theory of EDAs) LeadingOnes

SUBSTRING(x) =
$$\begin{cases} 2n & \text{if } x = (1, \dots, 1) \\ \max_{i=1}^{n} i \cdot \prod_{j=\max\{i-n/4,1\}}^{i} x_j & \text{otherwise} \end{cases}$$

SUBSTRING equals LEADINGONES if no block of at least n/4 consecutive ones. E.g.: 11110 * * * * * * * * + + 4

Otherwise, it describes the starting position of the rightmost block of n/4 ones – except if everything is one. E.g.: 010101011...111 $\mapsto 3n/4$

heory of EDAs) LeadingOnes

EDAS BEAT EAS ON SUBSTRING

Theorem (simplified from Chen et al., 2009a)

(1+1) EA needs with overwhelming probability time 2^{cn} to optimize SUBSTRING. UMDA with $\lambda = \Omega(n^{2+\varepsilon})$, $\mu = \lambda/2$ optimizes SUBSTRING in polynomial time w. o. p.

(1+1) EA

 $\begin{array}{l}t \leftarrow 0;\\ \mathsf{Draw} \ x_0 \in \{0,1\}^n \ \text{uniformly at random};\\ \textbf{while termination criterion not met do}\\ \\ \mathsf{Create} \ y \ \text{by flipping each bit in } x_t \ \text{independently with prob. } 1/n;\\ \textbf{if } f(y) \geq f(x_t) \ \textbf{then } x_{t+1} \leftarrow y;\\ \textbf{else } x_{t+1} \leftarrow x_t;\\ t \leftarrow t+1; \end{array}$

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Proof idea for (1+1) EA

When > n/4 leading ones, the first bit(s) no longer contributes to fitness. These bits slowly become random again. Optimum missed, NIAH

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Theory of EDAs > LeadingOnes

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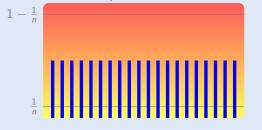
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Proof idea for UMDA

Also UMDA starts out by gaining more and more leading ones. This is reflected in the frequencies.



10101110110111011010

Even after the first bits no longer contribute to fitness, their frequencies are **expected** to remain the same. All-ones string can be sampled.

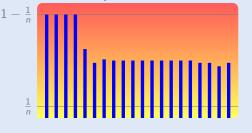
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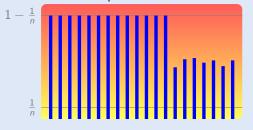


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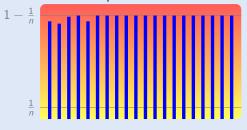
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LEADINGONES: SUMMARY	CONTENTS
	Introduction
	Preliminarie
Typical behavior of EDAs: ▶ On ONEMAX they optimize all bits roughly at the same time.	OneMax
 On LEADINGONES they optimize bits from left to the right. 	LeadingOne
• Runtime $\Theta(n \log n)$ vs. $\Theta(n^2)$ for opt. parameters settings.	BinaryValue
	Noise
However, there are other EDAs that do not behave like this (see later).	lump
	Jump
	Stable EDAs

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e

THE FINAL EXAMPLE FUNCTION: BINVAL

Recall

$$\operatorname{BINVAL}(x_1,\ldots,x_n) := \sum_{i=1}^n 2^{n-i} x_i,$$

being somewhere between $\rm LEADINGONES$ and $\rm ONEMAX.$ A bit outweighs all less significant bits together, but every bit contributes to fitness.

Often, a runtime analysis of LEADINGONES also gives a runtime bound for BINVAL (e.g., for UMDA/PBIL, Lehre and Nguyen, 2018).

Theorem (Droste, 2006)

The runtime of cGA on BINVAL is O(Kn) for $K = \Omega(n^{1+\varepsilon})$ w.o. p. It is $\Omega(Kn)$ w.o. p.

Note: upper bound $O(n^{2+\varepsilon})$. Lower bound does not restrict K.

NOT ALL LINEAR FUNCTIONS ARE EQUALLY DIFFICULT FOR EDAS

Known for (1+1) EA (W., 2013): all linear functions optimized in expected time $(1 \pm o(1))en \ln n$.

 \Rightarrow Runtimes on ${\rm ONEMAX}$ and ${\rm BINVAL}$ differ by a lower-order term.

Droste conjectured that BINVAL cannot be optimized in time $O(n \log n)$.

Theorem (W., 2018)

The runtime of cGA (without borders) on BINVAL is $\Omega(n^2)$ with prob. $\Omega(1)$. Choosing K = o(n) leads to infinite runtime w. h. p.

Idea: if K too small, genetic drift likely to occur at light bits before all heavy bits optimized.

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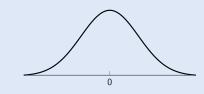
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Optimization under Uncertainty

Assume that an evaluation of the objective function is subject to random noise.

Example: ONEMAX with additive Gaussian noise

$$f_{\text{noise}}(x) = \text{ONEMAX}(x) + N(0, \sigma).$$



Typical measures to handle noise in evolutionary computation:

- large populations
- resampling
- ▶ ...

Theory of EDAs) Noise

EDAs have a built-in noise handling mechanism.

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neory of EDAs) Noise

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Theory of EDAs) Noise

EDAS BEAT POPULATION-BASED EAS IN NOISY SETTINGS

Definition (Friedrich et al., 2017): an algorithm scales gracefully if its expected runtime depends polynomially on the noise strength. For example: runtime is proportionally to σ^2 .

Theorem

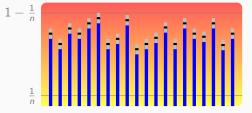
 $(\mu+1)$ EA does not scale gracefully on ONEMAX with additive Gaussian noise. However, cGA does.

PROOF IDEAS

• $(\mu+1)$ EA uses mutation, which drifts away from the optimum when there are many correct bits and noise disturbs fitness signal.

 $\operatorname{Prob}(f(x) > f(y)) \approx \operatorname{Prob}(f(x) < f(y))$

cGA does not use mutation and is *balanced*: in expectation, frequency vector and thus fitness does not decrease over time.



- cGA does not receive negative signal from noise, but signal (drift) towards increasing ONEMAX becomes smaller with increasing σ .
- ▶ Have to ensure that effect of genetic drift is smaller than the signal \rightarrow choose big enough K.

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heory of EDAs) Noise

FURTHER NOISY SETTINGS

Also simple ACO algorithms can be considered EDAs and are superior to EAs in some noisy settings (also from combinatorial optimization):

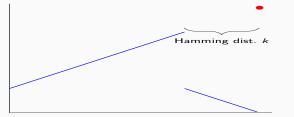
- ▶ Sudholt and Thyssen (2012) for ACO for noisy shortest paths with a ground truth
- ▶ Doerr et al. (2012) where the noise is intrinsic
- ► Feldmann and Kötzing (2013) for ACO with fitness-proportional updates: leads to convergence to expected best solution

Many of the results can probably be transferred to more classical EDAs such as cGA and UMDA.

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How EDAs Overcome Gaps

JUMP challenging for hillclimbers: $\Theta(n^k)$ to cross gap of size k > 1.



EDAs can search more globally in Jump region thanks to higher sampling variance \rightsquigarrow time $\Theta(c^k)$ instead of $\Theta(n^k)$ (first observed in Hasenöhrl and Sutton, 2018).

Theorem (Doerr, 2019)

If $k \leq \frac{1}{20} \ln n$ and $\mu = \Omega(\sqrt{n} \log n)$ then cGA optimizes Jump in $O(\mu\sqrt{n})$ iterations w. h. p. Time $O(n \log n)$ if $\mu = \Theta(\sqrt{n} \log n)$.

See talk at this GECCO.

neory of EDAs) Stable EDAs

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heory of EDAs) Stable EDAs

BALANCEDNESS, STABILITY AND GENETIC DRIFT

Have seen: without fitness signal, stochastic model of EDAs is expected to be the same. Term: balanced (Friedrich et al., 2016a).

However, this is only the *expected value*. Genetic drift plays major role in classical EDAs.



Term: EDA is stable if a frequency in absence of fitness signal stays close to its initial value.

cGA, UMDA, ... are not stable. Frequencies quickly converge to either maximum or minimum (each with probability 1/2) due to genetic drift.

Theory of EDAs) Stable EDAs

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A New Way to Overcome Genetic Drift: Significance-Based EDAs

Idea (Doerr and Krejca, 2018): Move frequency away from its initial value only when there is evidence that 0 or 1 is the better bit value.

sig-cGA: algorithmic ideas

- Framework like cGA.
- ▶ For each bit, history $H_i \in \{0,1\}^*$ of values in better individual
- ► Investigate last *m* history bits. If a value significantly dominates, move frequency to corresponding border (1/n if 0 dominates, 1 1/n if 1).
- ▶ Otherwise, leave frequency at 1/2.
- Example of significance: $|||H_i||_1 \frac{m}{2}| \ge C\sqrt{m \ln n}$
- ▶ Different values for *m* are tested by the algorithm.

SIGNIFICANCE-BASED EDAS ARE FAST

Theorem

The expected runtime of sig-cGA on both ONEMAX ond LEADINGONES is $O(n \log n)$ (and with high probability).

No other evolutionary algorithm is known that simultaneously optimizes ONEMAX and LEADINGONES in time $O(n \log n)$.

Proof ideas

- On ONEMAX, drift Ω(p_i(1 − p_i)/√n) quickly identified as significant. Many ideas of analysis of plain cGA work.
- On LEADINGONES, frequencies are optimized from left to right. Bits that do not contribute to fitness yet: no signal, no significance of deviation, no genetic drift, stay at 1/2

Significance-based EDAs are promising, theory-driven approach.

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SUMMARY AND CONCLUSIONS

Summary

- Runtime analysis for simple univariate EDAs
- Identified similarities to and differences from simple EAs
- Genetic drift a major obstacle
- Sensitive to parameters (phase transitions)
- Robust to noise
- Significance-based EDAs as novel theory-driven approach

Future work

- Combinatorial problems
- Multivariate EDAs
- Classification of problems w. r. t. appropriateness for EAs/EDAs, ...

Book chapter related to this tutorial

Martin Krejca and Carsten Witt, Theory of Estimation-of-Distribution Algorithms, in: B. Doerr and F. Neumann (editors), Theory of Randomized Search Heuristics in Discrete Search Spaces, Springer, to appear

https://arxiv.org/abs/1806.05392

Thank you!

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