

Theory for Non-Theoreticians

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Link to the Latest Version

- We will most likely update the slides between the proceedings submission deadline in May and the tutorial in July.
- You can always find the latest version online at <http://people.mpi-inf.mpg.de/~doerr/GECCO16tutorial.pdf>

Instructors 1/2: Benjamin Doerr

- **Benjamin Doerr** is a full professor at the French École Polytechnique.
- He received his diploma (1998), PhD (2000) and habilitation (2005) in mathematics from Kiel University. His research area is the theory both of problem-specific algorithms and of randomized search heuristics like evolutionary algorithms. Major contributions to the latter include runtime analyses for evolutionary algorithms and ant colony optimizers, as well as the further development of the drift analysis method, in particular, multiplicative and adaptive drift. In the young area of black-box complexity, he proved several of the current best bounds.
- Together with Frank Neumann and Ingo Wegener, Benjamin Doerr founded the theory track at GECCO, served as its co-chair 2007-2009 and serves again in 2014. He is a member of the editorial boards of *Evolutionary Computation*, *Natural Computing*, *Theoretical Computer Science*, *Journal of Complexity*, *RAIRO Theoretical Informatics and Applications*, and *Information Processing Letters*. Together with Anne Auger, he edited the book *Theory of Randomized Search Heuristics*.

Instructors 2/2: Carola Doerr

- **Carola Doerr, née Winzen**, is a permanent researcher with the CNRS and the Université Pierre et Marie Curie (Paris 6). Her main research interest is in the theory of randomized search heuristics, both in the design of efficient algorithms as well as in lower bounds for such general-purpose optimization techniques.
- She studied mathematics at Kiel University (Diploma in 2007) and computer science at the Max Planck Institute for Informatics and Saarland University (PhD in 2011). Her PhD studies were supported by a Google Europe Fellowship in Randomized Algorithms. From Dec. 2007 to Nov. 2009, Carola Doerr has worked as a business consultant for McKinsey & Company. She was a post-doc at the Université 7 in Paris and the Max Planck Institute for Informatics in Saarbrücken.
- Carola has been co-chair of the theory track at GECCO 2015 and serves as tutorial chair at PPSN 2016. She is editor of a special issue in *Algorithmica* and is since 2014 a co-organizer of the women@GECCO workshop series.

Target Audience & Objectives of This Tutorial

- This tutorial addresses GECCO attendees who do not regularly use mathematical proofs in their everyday research activities
- We want to help you understanding
 - what theory of evolutionary computation (EC) is
 - how it shapes our understanding of EC
 - how to read and understand theory results
 - what type of results to expect from theory (and which not)
 - and give an overview of some “hot topics” in the theory of EC
- We do **NOT** want to
 - deliver an introductory tutorial on theory of EC, runtime analysis,... for researchers interested in doing theory analyses themselves
 - discuss any mathematical techniques or recent results or promising research questions in the theory of EC or ...

Modus Operandi

- We have prepared a slide presentation but this should not stop you from starting discussions or commenting on the content of this tutorial → the more you get involved, the more we can learn from each other (and the more fun it is for all of us)
- Don't hesitate to ask questions during the tutorial!
(if we are using a phrase that you do not know it is likely that someone else in the room does not know it either, same if we are unable to get our message across)
- This is the first time that we are presenting this tutorial at GECCO and we are hence grateful for any kind of feedback on this tutorial (e.g., during the coffee breaks, receptions, via email, ...), so please let us know if it was useful for you and what you would like to see changed for future editions of this tutorial!

Outline of the Tutorial

- **Part I:** What We Mean by *Theory of EC*
 - We discuss the main differences between theory and other forms of research in evolutionary computation
- **Part II:** A Guided Walk Through a Famous Theory Result
 - We use an illustrative example to explain how to read and interpret a typical theory result
 - We also discuss limitations of theoretical research
- **Part III:** How Theory Has Contributed to a Better Understanding of EAs
 - 3 examples showing how theory can have an impact
- **Part IV:** Current Hot Topics in the Theory of EAs
- **Part V:** Concluding Remarks
- **Appendix:** glossary, references

Focus on EAs with Discrete Search Spaces

- To not overload you with definitions and notation, we only cover theory for *evolutionary algorithms* on *discrete search spaces*.
- Hence we intentionally omit
 - genetic programming, estimation of distribution algorithms, ant colony optimizers, swarm intelligence, ...
 - all optimization of continuous functions
- There is strong theory research in these areas
- All main messages of this tutorial are equally valid for these areas
 - so we “only” omit examples from these areas

Part I:

What We Mean by “Theory of EC”

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What Do We Mean With *Theory*?

- Definition (for this tutorial):
By theory, we mean results proven with mathematical rigor
- Mathematical rigor:
 - make precise the evolutionary algorithm (EA) you regard
 - make precise the problem you try to solve with the EA
 - make precise a statement on the performance of the EA solving this problem
 - prove this statement
- **Example:**
Theorem: The (1+1) EA finds the optimum of the OneMax test function $f: \{0,1\}^n \rightarrow \mathbb{R}; x \mapsto \sum_{i=1}^n x_i$ in an expected number of at most $en \ln(n)$ iterations.
Proof: blah, blah, ...

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Other Notions of Theory

- **Theory:** Mathematically proven results
 =====<in this tutorial, we focus on the above>=====
- **Experimentally guided theory:** Set up an artificial experiment to experimentally analyze a particular question
 - example: add a neutrality bit to two classic test functions, run a GA on these, and derive insight from the outcomes of the experiments
- **Descriptive theory:** Try to describe/measure/quantify observations
 - example: parts of landscape analysis
- **“Theories”:** Unproven claims guiding our thinking
 - example: building block hypothesis

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Why Do Theory? Because of Results

- Absolute guarantee that the result is correct
 - for yourself
 - for reviewers and journal
 - for the reader of your papers: anyone with moderate maths skills can fully check your result
- Many results can only be obtained by theory; e.g., because you make a statement on a very large or even infinite set
 - all bit-strings of length n ,
 - all TSP instances on n vertices,
 - all input sizes $n \in \mathbb{N}$,
 - all possible algorithms for a problem

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Why Do Theory? Because of the Approach

- A proof (automatically) gives insight in
 - how things work (→ working principles of EC)
 - why the result is as it is
- Self-correcting/self-guiding effect of proving: when proving a result, you are automatically pointed to the questions that need more thought
- Trigger for new ideas
 - clarifying nature of mathematics
 - playful nature of mathematicians

The Price for All This

Theory results are very true, very trustworthy, very exact. This comes at a price... Possible drawbacks include:

- Restricted scope: So far, mostly simple algorithms could be analyzed for simple optimization problems
- Less precise results: Constants are not tight, or not explicit as in " $O(n^2)$ " = "less than cn^2 for some unspecified constant c "
- Less specific results: You get a weaker guarantee for all problem instances instead of a stronger one for the practically more relevant instances
- Theory results can be very difficult to obtain: The proof might be short and easy to read, but finding it took long hours

Theory and Experiments: Complementary Results

THEORY

- cover all problem instances of arbitrary sizes
→ guarantees
- proof tells you the reason
- only models for real-world instances, and even this is hard
- limited scope
- limited precision
- implementation independent
- finding proofs can be difficult

EXPERIMENTS

- only a finite number of instances of bounded size
→ have to hope that this is representative
- only tells you numbers
- real-world instances
- everything you can implement
- exact numbers
- depends on implementation
- often cheap to do

→ Ideal: Combine theory and experiments. Difficulty: Get good theory people and good experimental people to talk to each other...

Part II: A Guided Walk Through a Famous Theory Result

Outline for This Part

- We use a simple but famous theory result
 - as an example for a non-trivial result
 - to show how to read a theory result
 - to explain the meaning of such a theoretical statement
 - to discuss typical shortcomings of theory results

A Famous Result

Theorem: The (1+1) evolutionary algorithm finds the maximum of any linear function

$$f: \{0,1\}^n \rightarrow \mathbb{R}, (x_1, \dots, x_n) \mapsto \sum_{i=1}^n w_i x_i, \quad w_1, \dots, w_n \in \mathbb{R},$$

in an expected number of $O(n \log n)$ iterations.

Reference: This is Theorem 12 in

[DJW02] S. Droste, T. Jansen, and I. Wegener. On the analysis of the (1+1) evolutionary algorithm. Theoretical Computer Science, 276(1-2):51-81, 2002.

Reading This Result

(1+1) evolutionary algorithm to maximize $f: \{0,1\}^n \rightarrow \mathbb{R}$:

1. choose $x \in \{0,1\}^n$ uniformly at random
2. while not terminate do
3. generate y from x by flipping each bit independently with probability $1/n$ ("standard-bit mutation")
4. if $f(y) \geq f(x)$ then $x := y$
5. output x

A mathematically proven result

Theorem: The (1+1) evolutionary algorithm finds the maximum of any linear function

$$f: \{0,1\}^n \rightarrow \mathbb{R}, (x_1, \dots, x_n) \mapsto \sum_{i=1}^n w_i x_i, \quad w_1, \dots, w_n \in \mathbb{R},$$

in an expected number of $O(n \log n)$ iterations.

A hidden all-quantifier: we claim the result for all $w_1, \dots, w_n \in \mathbb{R}$

At most $Cn \ln n$ for some unspecified constant C

Performance measure: number of iterations (not runtime in seconds)

What is Cool About This Result?

- Gives a *proven* performance guarantee
- General: A statement for *all* linear functions in *all* dimensions n
- Non-trivial
- Surprising
- Provides insight in how EAs work

→ more on these 3 items on the next slides

Theorem: The (1+1) evolutionary algorithm finds the maximum of any linear function

$$f: \{0,1\}^n \rightarrow \mathbb{R}, (x_1, \dots, x_n) \mapsto \sum_{i=1}^n w_i x_i, \quad w_1, \dots, w_n \in \mathbb{R},$$

in an expected number of $O(n \log n)$ iterations.

Non-Trivial: Hard to Prove & Hard to Explain Why it Should be True

▪ Hard to prove

- 7 pages complicated maths proof in [DJW02]
- we can do it in one page now, but only because we developed a deep technique for the analysis of such problems (drift analysis)

▪ No “easy” explanation

- *monotonicity* is not enough: if the w_i are all positive, then “flipping a 0 to a 1 always increases the fitness” (monotonicity).
 - easy explanation that is not true: monotonic functions are easy to optimize for an EA – disproved in [DJS⁺13]
- *separability* is not enough
 - a linear function can be written as a sum of functions f_i such that the f_i depend on disjoint sets of bits
 - also wrong: the optimization time of such a sum is not much more than the worst optimization time of the summands (because the independent f_i are optimized in parallel) – disproved in [DSW13]

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Surprising: Same Runtime For Very Different Fitness Landscapes

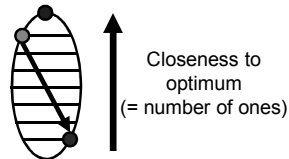
- **Example 1:** OneMax, the function counting the number of 1s in a string, can be written as $OM: \{0,1\}^n \rightarrow \mathbb{R}, (x_1, \dots, x_n) \mapsto \sum_{i=1}^n x_i$
- For OneMax, we easily see that the unique global maximum is $(1, \dots, 1)$, having a fitness of n
- We also see that the larger the fitness value of a string is, the closer it is to the optimum $(1, \dots, 1)$. In fact, there is a 1:1 correspondence between the fitness distance and structural distance to the optimum. OneMax therefore looks like an easy to optimize function
- **Example 2:** BinaryValue (BinVal or BV for short), the function mapping a binary string to the decimal number it represents, i.e., $BV: \{0,1\}^n \rightarrow \mathbb{R}, (x_1, \dots, x_n) \mapsto \sum_{i=1}^n 2^{n-i} x_i$
- Low fitness-distance correlation (see next slide)

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Comparison of OneMax and BinVal

- $OM(000) = 0 = BV(000)$
- $OM(001) = 1 = BV(001)$
- $OM(100) = 1$ and $BV(100) = 4$
- $OM(011) = 2$ and $BV(011) = 1 + 2 = 3 < 4 = BV(100)$
- Note here that the string (011) is closer to the optimum (111) than the string (100), but it has smaller BV-fitness
- In general, $BV(01..1) = \sum_{i=2}^n 2^{n-i} = 2^{n-1} - 1 < 2^n = BV(10..0)$
- This shows that for BinVal (unlike for OneMax) there is not such a nice 1:1 correlation between distance to the optimum and fitness values
- The (1+1) EA prefers 10..0 over 01...1 and may therefore move away from the target during the optimization process



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Insight in Working Principles

- Insight from the result:
 - Even if there is a low fitness-distance correlation (as is the case for the BinVal function), EAs can be very efficient optimizers
- Insight from the proof:
 - The fitness has very little influence on the quality of a search point!
 - Despite the large variety of linear functions, for all linear functions the quality of a search point is well approximated by its Hamming distance $H(x, x^*)$ to the optimum:
 - If the current search point of the (1+1) EA is x , then the optimum is found within an expected number of at most

$$4en \ln(2eH(x, x^*))$$

iterations (independent of f).

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A Glimpse on a Modern Proof

- **Theorem [DJW12]:** For all problem sizes n and all linear functions $f: \{0,1\}^n \rightarrow \mathbb{R}$ with $f(x) = w_1x_1 + \dots + w_nx_n$ the (1+1) EA finds the optimum of f in an expected number of at most $4en \ln(2en)$ iterations.
- **1st proof idea:** Without loss, we can assume that $w_1 \geq w_2 \geq \dots \geq w_n > 0$
- **2nd proof idea:** Regard an artificial fitness measure!
 - Define $\tilde{f}(x) = \sum_{i=1}^n \left(2 - \frac{i-1}{n}\right) x_i$ “artificial weights from $1 + \frac{1}{n}$ to 2^n ”
 - Key lemma: Consider the (1+1) EA optimizing the original f . Assume that some iteration starts with the search point x and ends with the random search point x' . Then

$$E[\tilde{f}(x^*) - \tilde{f}(x')] \leq \left(1 - \frac{1}{4en}\right) (\tilde{f}(x^*) - \tilde{f}(x))$$

“expected artificial fitness distance reduces by a factor of $\left(1 - \frac{1}{4en}\right)^n$ ”
- **3rd proof idea:** Multiplicative drift theorem translates this expected progress w.r.t. the artificial fitness into a runtime bound
 - roughly: the expected runtime is at most the number of iterations needed to get the artificial fitness distance below one.

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Multiplicative Drift Theorem

- **Theorem [DJW12]:** Let X_0, X_1, X_2, \dots be a sequence of random variables taking values in the set $\{0\} \cup [1, \infty)$. Let $\delta > 0$. Assume that for all $t \in \mathbb{N}$, we have $E[X_{t+1}] \leq (1 - \delta)E[X_t]$. Let $T := \min\{t \in \mathbb{N} \mid X_t = 0\}$. Then

$$E[T] \leq \frac{1 + \ln X_0}{\delta}$$
- On the previous slide, this theorem was used with
 - $\delta = 1/4en$
 - $X_t = \tilde{f}(x^*) - \tilde{f}(x^{(t)})$
 - and the estimate $X_0 \leq 2n$.
- **Bibliographical notes:** Artificial fitness functions very similar to this \tilde{f} were already used in [DJW02] (conference version [DJW98]). Drift analysis (“translating progress into runtime”) was introduced to the field in [HY01] to give a simpler proof of the [DJW02] result. A different approach was given by [Jäg08]. (Variants of) the multiplicative drift theorem [DJW12] (conference version [DJW10]) is one of the most-used drift theorems today.

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What is Uncool About This Result?

- An unrealistically simple EA: the (1+1) EA
 - Linear functions are simple
 - Not a precise result, but only $O(n \log n)$ in [DJW02] or a most likely significantly too large constant in the [DJW10] result just shown
- We discuss these points on the following slides

Theorem: The (1+1) evolutionary algorithm finds the maximum of any linear function

$$f: \{0,1\}^n \rightarrow \mathbb{R}, (x_1, \dots, x_n) \mapsto \sum_{i=1}^n w_i x_i, \quad w_1, \dots, w_n \in \mathbb{R},$$

in an expected number of $O(n \log n)$ iterations.

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Maybe Uncool: Only the Simple (1+1) EA

- This was, at that time (2002), the absolute maximum that was possible when asking for a proven result.
- Today, we know (a little bit) more. E.g., the $(1 + \lambda)$ EA optimizes any linear function in time (= number of fitness evaluations)

$$O(n \log n + \lambda n).$$

This bound is sharp for BinVal, but not for OneMax, where the optimization time is

$$O\left(n \log n + \lambda n \frac{\log \log \lambda}{\log \lambda}\right).$$

→ Not all linear functions have the same optimization time! [DK15]

- We are optimistic that the theory community will make progress towards more complicated EAs

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Maybe Uncool: Only Linear Functions

- Again, this was the starting point. Today, we know how the (1+1) EA (and some other algorithms) compute
 - Eulerian cycles [Neu04,DHN06,DKS07,DJ07]
 - shortest paths [STW04,DHK07,BBD⁺09]
 - minimum spanning trees [NW07,DJ10,Wit14]
 - and many other “easy” optimization problems
- We also have some results on approximate solutions for NP-complete problems like Partition [Wit05], vertex cover [FHH⁺09,OHY09], maximum cliques [Sto06]
- We are optimistic that we will enlarge the set of problems we understand. However, it is also clear that “theory will always be behind”; that is, it will take quite some time until theoretical analyses become available for typical algorithms used in practice and realistic real-world problems (this is partially due to the fact that EAs are most typically used in situations that are extremely difficult to analyze as for “easy” problems, the design of a problem-tailored algorithm is a preferred approach)

Maybe Uncool: $O(n \log n)$, Large Constant

- Having only asymptotic results is a typical price for proven results (also in the classic algorithms field).
- There is the general experience that often a proven “ $O(n \log n)$ ” in fact means “roughly $cn \log n$ ” for a small constant c , which can, e.g., be obtained from experiments
- We know more now [Wit13]: The runtime of the (1+1) EA on any linear function is $en \ln n + O(n)$, that is, at most $en \ln n + Cn$ for some constant C
 - still an asymptotic result, but the asymptotics are only in a lower order term
 - [Wit13] also has a non-asymptotic result, but it is hard to digest

Theorem 4.1. *On any linear function on n variables, the optimization time of the (1+1) EA with mutation probability $0 < p < 1$ is at most*

$$(1-p)^{1-n} \left(\frac{nx^2(1-p)^{1-n}}{\alpha-1} + \frac{\alpha}{\alpha-1} \frac{\ln(1/p) + (n-1)\ln(1-p) + r}{p} \right) =: b(r),$$

with probability at least $1 - e^{-r}$ for any $r > 0$, and it is at most $b(1)$ in expectation, where $\alpha > 1$ can be chosen arbitrarily (even depending on n).

Part III:

How Theory Can Contribute to a Better Understanding of EAs

Outline for This Part

3 ways how theory can help understanding and improving EAs

1. Debunk misconceptions
2. Help choosing the right parameters, representations, operators, and algorithms
3. Invent new representations, operators, and algorithms

Contribution 1: Debunk Misconceptions

- When working with EA, it is easy to conjecture some general rule from observations, but (without theory) it is hard to distinguish between “we often observe” and “it is true that”
- Reason: it is often hard to falsify a conjecture experimentally
 - the conjecture might be true “often enough” or for the problems we just have in mind, but not in general
- Danger: misconceptions prevail in the EA community and could mislead the future development of the field
- 2 (light) examples on the following slides

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Misconception: Functions Without Local Optima are Easy to Optimize

- A function $f: \{0,1\}^n \rightarrow \mathbb{R}$ has *no local optima* if each non-optimal search point has a neighbor with better fitness
 - if $f(x)$ is not maximal, then by flipping a single bit of x you can get a better solution
- Misconception: Such functions are easy to optimize...
 - because already a simple hill-climber flipping single bits (randomized local search) does the job
- Truth: There are functions without local optima where several common EAs with high probability need exponential (in n) time to find the optimum (or even a reasonable good solution) [HGD94,Rud97,DJW98]
 - reason: yes, it is easy to find a better neighbor if you're not optimal yet, but you may need to do this an exponential number of times because all improving paths to the optimum are that long

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Misconception: Monotonic Functions are Easy to Optimize

- A function $f: \{0,1\}^n \rightarrow \mathbb{R}$ is monotonically strictly increasing if the fitness increases whenever you flip a 0-bit to 1
 - special case of “no local optima” where each neighbor with more ones is better
- Misconception: Such functions are easy to optimize for standard EAs...
 - because already a simple hill-climber flipping single bits (randomized local search) does the job in time $O(n \log n)$
- [DJS⁺13]: There is a monotonically strictly increasing function such that with high probability the (1+1) EA with mutation probability $16/n$ needs exponential time to find the optimum
 - very different from linear functions with positive weights: $O(n \log n)$ time

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Summary Misconceptions

- Intuitive reasoning or experimental observations can lead to wrong beliefs.
- It is hard to falsify them experimentally, because
 - counter-examples may be rare (so random search does not find them)
 - counter-examples may have an unexpected structure
- There is nothing wrong with keeping these beliefs as “rules of thumb”, but it is important to distinguish between what is a rule of thumb and what is a proven fact
 - Theory is the right tool for this!

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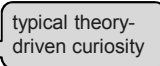
Contribution 2: Help Designing EAs

- When designing an EA, you have to decide between a huge number of design choices: the basic algorithm, the operators and representations, and the parameter settings.
- Theory can help you with deep and reliable analyses of scenarios similar to yours
 - The question “what is a similar scenario” remains, but you have the same difficulty when looking for advice from experimental research
- 3 examples:
 - fitness-proportionate selection
 - edge-based representations for optimization problems in graphs
 - use of crossover

Designing EAs: Fitness-Proportionate Selection

- Fitness-proportionate selection has been criticized (e.g., because it is not invariant under re-scaling the fitness), but it is still used a lot.
- Theorem [OW15]: If you use
 - the Simple GA as proposed by Goldberg [Gol89] (fitness-proportionate selection, comma selection)
 - to optimize the OneMax test function $f: \{0,1\}^n \rightarrow \mathbb{R}; x \mapsto x_1 + \dots + x_n$
 - with a population size $n^{0.2499}$ or less
 then with high probability the GA in a polynomial number of iterations does not create any individual that is 1% better than a random individual
- Interpretation: Most likely, fitness-proportionate selection and comma selection together make sense only in rare circumstances
 - more difficulties with fitness-proportionate selection: [HJKN08, NOW09]

Designing EAs: Representations

- Several theoretical works on shortest path problems [STW04, DHK07, BBD*09], all use a vertex-based representation:
 - each vertex points to its predecessor in the path
 - mutation: rewire a random vertex to a random neighbor
- [DJ10]: How about an edge-based representation? 
 - individuals are set of edges (forming reasonable paths)
 - mutation: add a random edge (and delete the one made obsolete)
- **Result:** All previous algorithms become faster by a factor of $\approx \frac{|V|^2}{|E|}$
 - [JOZ13]: edge-based representation also preferable for vertex cover
- Interpretation: While there is no guarantee for success, it may be useful to think of an edge-based representation even when a vertex-based representation looks more natural

Designing EAs: Do We Need Crossover?

“Eternal” debate: What is the role of crossover in EC?

- Applied work: Using crossover and mutation together seem to work well
- Holland’s [Hol75] building block hypothesis (BBH):
 - A genetic algorithm works by combining short, low-order, highly fit schemata (“building blocks”) into fitter higher order schemata
- Forrest, Mitchell [FM92]: Disprove BBH experimentally
 - design a simple optimization problem that perfectly fulfills the BBH
 - experiments: a simple hill-climber is much faster than a standard crossover-based algorithm

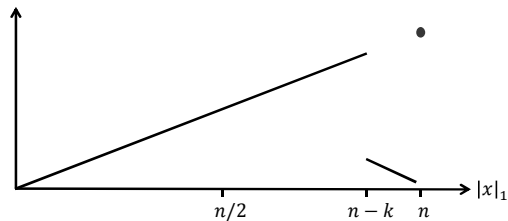
What can theory add to this debate?

- Possible first tiny step: Identify a problem and a reasonable EA such that the EA with crossover solves this problem better than without

Crossover: First Theory Attempt

Jansen&Wegener [JW99]: Jump functions

- fitness of an n -bit string x is the number of ones, except if this is in $\{n - k, \dots, n - 1\}$, then the fitness is the number of zeroes.



- Hope: One quickly finds many bit-strings with $n - k$ ones, then crossover combines two of these into the optimum $x^* = (1 \dots 1)$
- Analysis: Mutation needs $\Theta(n^k)$ iterations. With uniform crossover $O(n^2 \log n)$ suffice, but only for artificially small crossover rates ($\leq 1/n$)

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More Theory Results on Crossover

- [JW99] inspired a sequence of follow-up works ...
 - Jansen and Wegener [JW05] present artificial problems for which a GA with crossover is exponentially faster than mutation-based EAs
 - Storch and Wegener [SW04] show the same for population size 2
 - Fischer and Wegener [FW04], Sudholt [Sud05] show advantages of crossover in a simplified Ising model (all edge weights one \rightarrow constant spin assignment is the unique optimum)
- ... but all regard quite artificial problems
 - "It will take many major steps to prove rigorously that crossover is essential for typical applications." (Jansen and Wegener [JW05])
- Possible insight: If it is so hard to find a single convincing problem where crossover provably helps, maybe crossover is not so important?
 - At least, crossover is not easy to get to work, so maybe it is not the first choice when attacking a new problem

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Good News: Crossover Can Work

- First classic optimization problem where crossover provably gives a speed-up (of around a factor of \sqrt{n}): All-pairs shortest path problem \odot [DHK08, DT09, DJK⁺13]
 - proof also reveals why crossover works here: crossover finds some good solutions, mutation "fills the gaps" and finds the rest
 - not primarily "putting together of building blocks"
- Complexity theoretic view: Separation between mutation and crossover!
 - No unary unbiased black-box algorithm ("everything that uses only mutation and without cheating") can solve the OneMax problem faster than in roughly $n \ln n$ iterations [LW12, DDY16]
 - There is a binary unbiased black-box algorithm ("still no cheating, but generating an offspring from two parents is now allowed") solving the OneMax problem in $2n$ iterations [DJK⁺11]

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Contribution 3: New Algorithms (1/3)

- Theory can also, both via the deep understanding gained from proofs and by "theory-driven curiosity" invent new operators and algorithms. Here is one recent example:
- Theory-driven curiosity: Explain the following dichotomy!
 - the theoretically best possible black-box optimization algorithm \mathcal{A}^* for OneMax (and all isomorphic fitness landscapes) needs only $O(n/\log n)$ fitness evaluations
 - all known (reasonable) EAs need at least $n \cdot \ln n$ fitness evaluations
- One answer: \mathcal{A}^* profits from all search points it generates, whereas most EAs gain significantly only from search points as good or better than the previous-best
- Can we invent an EA that also gains from inferior search points?
 - YES [DDE15, DD15a, DD15b, Doe16], see next slides

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New Algorithms (2/3)

- A simple idea to exploit inferior search points (in a $(1+1)$ fashion):
 1. create λ mutation offspring from the parent by flipping λ random bits
 2. select the best mutation offspring ("mutation winner")
 3. λ times: biased uniform crossover of mutation winner with parent, taking bits from mutation winner with probability $1/\lambda$ only
 4. select the best crossover offspring ("crossover winner")
 5. elitist selection: crossover winner replaces parent if not worse
- Underlying idea:
 - If λ is larger than one, then the mutation offspring will often be much worse than the parent (large mutation rates are destructive)
 - However, the best of the mutation offspring may have made some good progress (besides all destruction)
 - Crossover with parent repairs the destruction, but keeps the progress

New Algorithms (3/3)

- Performance of the new algorithm, called $(1+(\lambda,\lambda))$ EA:
 - solves OneMax in time $O\left(\frac{n \log n}{\lambda} + \lambda n\right)$, which is $O(n \sqrt{\log n})$ for $\lambda = \sqrt{\log n}$
 - the parameter λ can be chosen dynamically imitating the 1/5th rule, this gives an $O(n)$ runtime
 - experiments:
 - these improvements are visible already for small values of λ and small problem sizes n
 - improvements also for other test problems
 - [GP14]: good results for satisfiability problems
- Interpretation: Theoretical considerations can suggest new algorithmic ideas. Of course, much experimental work and fine-tuning is necessary to see how such ideas work best for real-world problems.

Summary Part 3

Theory has contributed to the understanding and use of EAs by

- debunking misbeliefs (drawing a clear line between rules of thumb and proven fact)
 - e.g., "no local optima" does not mean "easy"
- giving hints how to choose parameters, representations, operators, and algorithms
 - e.g., how useful is crossover when we hardly find an example where it provably improves things?
- inventing new representations, operators, and algorithms; this is fueled by the deep understanding gained in theoretical analyses and "theory-driven curiosity"

Part IV: Current Topics of Interest in Theory of EC

What We Currently Try to Understand

- Precise runtime guarantees
- Population-based EAs
- Dynamic optimization, noisy environments
- Dynamic/adaptive parameter choices
- Non-elitism
- Black-box complexity
- Examples for these will be given on the next slides
- Parallel to these topics, we study also methodical questions (e.g., *drift analysis*), but these are beyond the scope of this tutorial

Precise Runtime Guarantees

- Theory results can give advice on how to choose the parameters of an EA
 - Example: the runtime often depends crucially on the mutation rate
- The more precisely we know the runtime (e.g., upper *and* lower bounds for its expected value), the more precise recommendations we can give for the right parameter choice
 - in practice, constant factors matter ☺
- Challenge: For such precise runtime bounds often the existing mathematical tools are insufficient
 - in particular, tools from classic algorithms theory are often not strong enough, because in that community (for several good reasons) there is no interest in bounds more precise than $O(\dots)$.

Precise Runtime Guarantees – Example

- [GW15]: The expected number of generations the $(1 + \lambda)$ EA with mutation rate c/n (c being a constant, λ not too large) takes to optimize OneMax, is

$$(1 \pm o(1)) \left(\frac{e^c}{c} \frac{n \log n}{\lambda} + \frac{1}{2} \frac{n \ln \ln \lambda}{\ln \lambda} \right)$$
- This result shows that for small λ , namely $\lambda = o(\ln n \ln \ln n / \ln \ln \ln n)$, the optimal mutation rate is $1/n$ (apart from lower order terms)
- For larger λ , namely $\lambda = \omega(\ln n \ln \ln n / \ln \ln \ln n)$, surprisingly, the mutation rate c/n does not have a significant influence on the expected runtime (as long as c is a constant)

Precise Runtime Guarantees – Where are We?

- We know the optimal mutation rates (apart from lower-order terms) for some classic simple EAs and test functions:
 - $1/n$ for the $(1+1)$ EA on linear functions [Wit13]
 - $1.59/n$ for the $(1+1)$ EA on the LeadingOnes test function [BDN10]
- We know that the runtime of the $(1+1)$ EA on OneMax reduces by $\Theta(\sqrt{n})$ iterations when we initialize with the best of two random individuals instead of just taking a random initial search point [dPdLDD15]
- Apart from this (and a few very specific results), we know nothing more precise than $O(\dots)$ -statements.
 - Is $1/n$ also the right mutation rate for most combinatorial optimization problems?
 - What is the influence of a constant-size parent and/or offspring population? [Usually no influence in $O(\dots)$ -land]

Population-Based EAs

- Population-based: using a non-trivial (≥ 2) population of individuals
- In practice, non-trivial populations are often employed
- In theory,
 - no convincing evidence (yet) that larger populations are generally beneficial (apart from making the algorithm easy to run on parallel machines)
 - the typical result is “up to a population size of ..., the total work is unchanged, for larger population sizes, you pay extra”
 - some evidence (on the level of artificially designed examples) that populations help in dynamic or noisy settings
 - not many methods to deal with the complicated population dynamics
- Big open problem: Give rigorous advice how to profitably use larger populations (apart allowing parallel implementations)
 - devise methods to analyze such algorithms

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Dynamic Optimization

- Dynamic optimization: Optimization under (mildly) changing problem data
- Question: How well do EAs find and track the moving optimum?
- First theory result [Dro02]: dynamic version of OneMax where the optimum changes (by one bit) roughly every K iterations
 - If $K = n/\log n$ or larger, then a polynomial number of iterations suffices to find or re-find the current optimum
 - K can be quite a bit smaller than the usual $en \ln n$ runtime!
 - First indication that EAs do well in dynamic optimization
- More recent results: Many (artificial) examples showing that populations, diversity mechanisms, island models, or ant colonies help finding or tracking dynamically changing optima [JS05,KM12,OZ15,LW14,LW15,...]
- Two main open problems: (i) What are realistic dynamic problems?
 - (ii) What is the best way to optimize these?

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Dynamic Parameter Choices

- Instead of fixing a parameter (mutation rate, population size, ...) once and forever (*static* parameter choice), it might be preferable to use parameter choices that change over time or depending on the performance (*dynamic* parameter choices).
- Hope:
 - different parameter settings may be optimal early and late in the optimization process
 - we do not need to know the optimal parameters beforehand, but the EA finds them itself
- Experimental work suggests that dynamic parameter choices often outperform static ones (for surveys see [EHM99,KHE15])

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Theory for Dynamic Parameter Choices

- Deterministic variation schedule* for the mutation rate: Huge runtime improvement for an artificial example function [JW06]
- Fitness-dependent* mutation rate: Constant factor speed-up over the best static mutation rate for the LeadingOnes test function [BDN10]
- Reduction of the parallel runtime (but not the total work) for several test functions when doubling the number of parallel instances in a parallel EA after each unsuccessful iteration (*success-based* dynamics) [LS11]
- [as discussed above] a success-based choice (1/5-th rule) of λ in the $(1+(\lambda, \lambda))$ GA gives the linear runtime on OneMax [DD15a], whereas all static parameter settings need at least roughly $n \sqrt{\log n}$ [DD15b,Doe16]
- State of the art: sporadic results, but very promising research direction
- Main research task: Gain some general understanding beyond particular examples when dynamic parameter settings are useful

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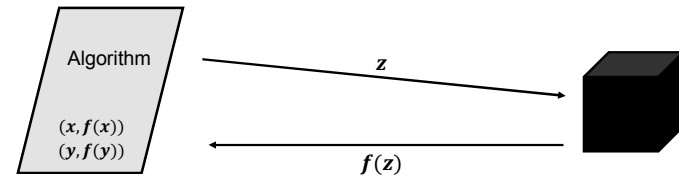
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Non-Elitism

- Most EAs analyzed in theory use *truncation selection*, which is an *elitist selection* = you cannot lose the best-so-far individual
- Mostly negative results on non-elitism are known. For example, [OW15] proves that the Simple Genetic Algorithm using *fitness-proportional selection* is unable to optimize OneMax efficiently [see above]
- Strong Selection Weak Mutation (SSWM) algorithm [PPHST15], inspired by an inter-disciplinary project with populations-genetics:
 - worsening solutions are accepted with some positive probability
 - for improving offspring, acceptance rate depends on the fitness gain
 - Examples are given in [PPHST15] for which SSWM outperforms classic EAs
- Black-box complexity view: there are examples where *any* elitist algorithm is much worse than a non-elitist algorithm [DL15]
- State of the art: Not much real understanding apart from sporadic results. The fact that non-elitism is used a lot in EC practice asks for more work.

Limits of EC: Black-Box Complexity

- EAs are *black-box algorithms*: they learn about the problem at hand only by evaluating possible solutions



- What is the price for such a problem-independent approach?
→ This is the main question in black-box complexity.
- In short, the black-box complexity of a problem is the minimal number of function evaluations that are needed to solve it
 - = performance of the best-possible black-box algorithm

Black-Box Complexity Insights

- Unified lower bounds: The black-box complexity is a lower bound for the runtime of *any* black-box algorithm: all possible kinds of EAs, ACO, EDA, simulated annealing, ...
- Specialized black-box models allow to analyze the impact of algorithmic choices such as type of variation in use, the population size, etc.
- Example result: [LW12] proves that every *unary unbiased* algorithm needs $\Omega(n \log n)$ function evaluations to optimize OneMax
 - unary: mutation only, no crossover
 - unbiased: symmetry in
 - bit-values 0 and 1
 - bit positions $1, 2, \dots, n$

→ Result implies that algorithms using fair mutation as only variation cannot be significantly more efficient on OneMax than the (1+1) EA

Part V: Conclusion

Summary

- Theoretical research gives deep insights in the working principles of EC, with results that are of a different nature than in experimental work
 - “very true” (=proven), but often apply to idealized settings only
 - *for all* instances, sizes, ..., but sometimes less precise
 - often only asymptotic results instead of absolute numbers
 - proofs also tell us *why* certain facts are true
- The different nature of theoretical and experimental results implies that a real understanding is best obtained from a combination of both
- *Theory-driven curiosity* and the *clarifying nature of mathematical proofs* can lead to new ideas, insights and algorithms

How to Use Theory in Your Work?

- Try to read theory papers, but don't expect more than from other papers
 - Neither a theory nor an experimental paper can tell you the best algorithm for your particular problem, but both can suggest ideas
- Try “theory thinking”: take a simplified version of your problem and imagine what could work and why
- Talk to the strange theory people ☺
 - yes, they speak a different language and they think differently
 - yes, they will not have the ultimate solution and their mathematical education makes them very cautious presenting an ultimate solution
 - but they might be able to prevent you from a wrong path or suggest alternatives to your current approach
 - and they (mostly) are very happy to discuss with non-theoreticians and see what the real world is like!

Recent Books (Written for Theory People, But Not Too Hard to Read)



- [AD11] Auger/Doerr 2011: Theory of Randomized Search Heuristics, World Scientific
- [Jan13] Jansen 2013: Analyzing Evolutionary Algorithms, Springer
- [NW10] Neumann/Witt 2010: Bioinspired Computation in Combinatorial Optimization, Springer

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Appendix A

Glossary of Terms Used in This Tutorial

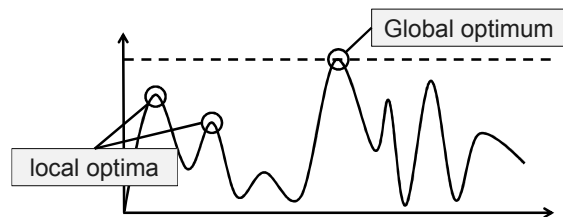
Discrete and Pseudo-Boolean Optimization

In this tutorial we are mostly interested in the optimization of problems of the type $f: \{0,1\}^n \rightarrow \mathbb{R}$

- Problems $f: S \rightarrow \mathbb{R}$ with finite search space S are called *discrete optimization problems* (in contrast to *continuous problems* $f: \mathbb{R}^n \rightarrow \mathbb{R}$ or, more generally $f: S \rightarrow \mathbb{R}$ with continuous S)
- When $S = \{0,1\}^n$ and $f: \{0,1\}^n \rightarrow \mathbb{R}$, we call f a *pseudo-Boolean function*
- Please note: don't get fooled! Even if optimizing a function $f: \{0,1\}^n \rightarrow \mathbb{R}$ may look harmless, a HUGE range of problems (even NP-hard ones like Max-SAT and many others!) can be expressed this way

What we Mean by “Optimization”

- Recall: we assume that we aim at optimizing a function $f: \{0,1\}^n \rightarrow \mathbb{R}$
- For this tutorial “optimization” = *maximization*, that is, we aim at finding a bit string $x = (x_1, \dots, x_n)$ such that $f(x) \geq f(y)$ for all $y \in \{0,1\}^n$
- Note in particular: we are not interested in this tutorial in identifying local optima, only the *global best solution(s)* are interesting for us



Expected Runtimes – Introduction

- All EAs are *randomized algorithms*, i.e., they use random decisions during the optimization process (for example, the *variation step*, i.e., the step in which new search points are generated, is often based on random decisions—we will discuss this in more detail below)
- Our object of interest, the *runtime of EAs*, is the number of function evaluations that an EA needs until it queries for the first time an optimal solution. Since EAs are randomized algorithms, their runtime is a random variable

Expected Runtimes – Definition

- Formally, let A be an EA, let f be a function to be optimized and let x^1, x^2, \dots be the series of search points queried by A in one run of optimizing f . The search points x^i are random and so is the series of fitness values $f(x^1), f(x^2), \dots$. The runtime T is defined by

$$T := \min \left\{ i \in \mathbb{N} \mid f(x^i) = \max_{y \in \{0,1\}^n} f(y) \right\}$$

- Several features of this random variable are interesting. We mostly care about the *expected runtime of an EA*. This number is the average number of function evaluations that are needed until an optimal solution is evaluated for the first time.
- Caution (1/2): sometimes runtime is measured in terms of *generations*, not *function evaluations*
- Caution (2/2): Regarding expectation only can be misleading (see next slide for an example), this is why we typically study also other features of the runtime, such as its concentration

Expected Runtimes – Caution!

- The expected runtime does not always tell you the full truth: There are functions for which the expected runtime is very large but which can be optimized in a small number of steps with a fair probability. Example: The DISTANCE function regarded in [DJW02], see next slide

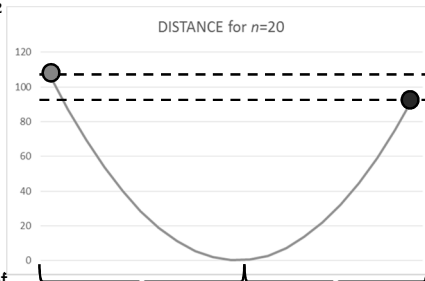
Expected Runtimes – Caution!

Formally,

$$\text{Distance}(x) := \left(\sum_{i=1, \dots, n} x_i - \frac{n}{2} - \frac{1}{3} \right)^2$$

We regard a simple hill climber (Randomized Local Search, RLS) which is

- initialized uniformly at random,
- flips one bit at a time,
- always accepts search points of best-so-far fitness



With probability (almost) 1/2, the algorithm has optimized DISTANCE after $O(n \log n)$ steps

With probability $\sim 1/2$ it does not find the optimum at all, thus having an infinite expected optimization time

Big-O Notation, aka Landau Notation (1/2)

- The “big-O” notation is used in algorithms theory to classify the order at which the running time of an algorithm grows with the size of the input problems
- In our example, it says that “The expected runtime of the (1+1) EA on any linear function with weights $\neq 0$ is $\Theta(n \log n)$.”
- $\Theta(n \log n)$ means that the expected runtime of the (1+1) EA on f is
 - $O(n \log n)$, that is, there exists a constant $C > 0$ such that for all n the expected runtime is at most $Cn \log n$
 - $\Omega(n \log n)$, that is, there exists a constant $c > 0$ such that for all n the expected runtime is at least $cn \log n$
- That is, there exist constants $0 < c < C$ such that

$$cn \log n \leq E(T_{(1+1)EA, f}) \leq Cn \log n$$

Big-O Notation, aka Landau Notation (2/2)

Further frequently used notation

- $f \in o(n)$ if f grows slower than linear. Formally:
for all constants $0 < c$ there exists a n_0 such that for all $n > n_0$: $f(n) \leq cn$
- $f \in \omega(n)$ if f grows faster than linear. Formally:
for all constants $0 < c$ there exists a n_0 such that for all $n > n_0$: $f(n) \geq cn$

Appendix B

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