Tutorial: Theory of Evolutionary Computation

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PPSN 2014, Ljubljana, Slovenia

Target for This Tutorial

- Give an introduction to EA theory aimed at an audience that is not working in theory already.
  - What is theory?
  - Why do theory?
  - How can the general EA community profit from theory?

- Feel free to ask questions at any time!

- We're happy to receive all kinds of feedback.

Outline

- [b10:35] Introduction: What do we mean by theory? Why? Why not?
- [b10:50] How theory can help understand EC: 3 examples
  - Warning: What looks easy might be difficult
  - Choosing good representations, operators, …
  - Do we need crossover?
- [a11:10] Basics: from discrete to continuous optimization
  - "interesting" theoretical questions and their relationship to practice
- [a11:30] Linear convergence of adaptive algorithms
  - illustrate benefits and limitation of theory wrt experiments
- [a11:50] Information geometry perspective
  - where theory sheds new light on "old" algorithms and gives new perspectives for algorithm design
- [b12:10] The F-words in theory

What Do We Mean With *Theory*?

- Definition (for this tutorial): By theory, we mean results proven with mathematical rigor and nothing else.

- Mathematical rigor:
  - make precise the 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: The (1+1) EA finds the optimum of the OneMax test function $f:\{0,1\}^n \to \mathbb{R}; x \mapsto \sum_{i=1}^{n} x_i$ in an expected number of at most $en\ln(n)$ iterations.
  Proof: blah, blah, …

Theory, Theories, and Everything Else

- Theory: Mathematically proven results
- 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

Theory, Theories, and Everything Else

- 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
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Why Do Theory? – 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

Why Do Theory? – 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 results, you are automatically pointed led 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 (e.g., (1+1) EA) on simple problems (test functions, “easy” graph problems) could be analyzed
- Less precise results: constants are not tight, or not explicit as in “$O(n^2)$” = “less than cn^2 for some unspecified constant c”
- More general than you want: You get a weaker statements for all problem instances instead of a strong one for the practically more relevant ones
- 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: Do both theory and experiments. Difficulty: Get good theory people and good experimental people to talk to each other…

What Can Theory Do For You? 3 Discrete Examples

max planck institut informatik

- Debunk misconceptions: What looks easy can be hard
- Give advice how to design EAs
- Contribute to the discussion how useful crossover is

Example 1: Prevent Misconceptions

- Misconception: Functions without local optimal are easy to optimize

- Horn, Goldberg, Deb (PPSN'94), Rudolph (1997), Droste, Jansen, Wegener (PPSN'98): There is a function $f\colon \{0,1\}^n \to \mathbb{R}$ such that
  - f has no local optima: If $f(x)$ is not maximal, then by flipping a single bit of x you can get a better solution
  - several common EAs need time exponential in n with high probability

- D.,Jansen, Sudholt, Winzen, Zarges (PPSN'10): There is a function $f\colon \{0,1\}^n \to \mathbb{R}$ such that
  - f is strictly monotonic: if you obtain y from x by flipping any zero to one, then $f(y) > f(x)$ [super-easy, no local optima, (1,…,1) is unique opt.]
  - the (1+1) EA with mutation probability $16/n$ needs time exponential in n with high probability

Example 2: Help in the Design of EA

- Example: Several theoretical works on shortest path problems
  - Scharnow, Tinnefeld, Wegener (PPSN'02)
  - D., Happ, Klein (CEC'07)
  - Baswana et al. (FOGA'09)

typical theory-driven curiosity

- All use a vertex-based representation:
  - each vertex points to its predecessor in the path
  - mutation: rewire a random vertex to a random neighbor
- D., Johannsen (GECCO'10): 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 $\approx \frac{|V|^2}{|E|}$

Example 2: Help in the Design of EA

- Theory result (proven, can be made precise): Going from a vertex-based to an edge-based representation speeds up several existing algorithms.

- Message beyond this particular result: Possibly, edge-based representations can be superior also for other graph problems

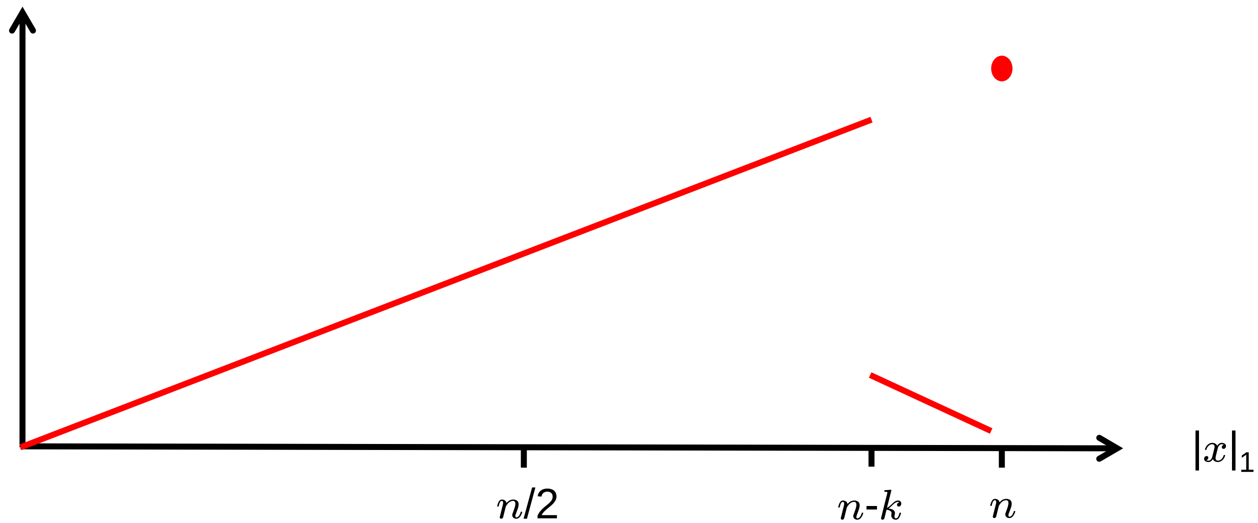
- Many more theory results giving advice/suggestions to the algorithm designer:
  - representations for the Eulerian cycle problem (where a permutation of edges is asked for)
  - optimal mutation probabilities
  - different selection mechanisms
  - …

Example 3: Do We Need Crossover?

- Applied work: Using crossover and mutation together seems to work well.
- Holland's (1975) 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 (1993): 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: Find a problem and a reasonable EA such that the EA with crossover performs better than without

First Theory Contribution

- Jansen&Wegener (1999): Jump functions.
  - fitness of an n-bit string x is the number of ones, except if this is in $\{n\text{-}k,\ldots,n\text{-}1\}$, 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^* = 11…..1
  - Analysis: Mutation needs $\Theta(n^k)$ iterations, with uniform crossover $O(n^2 \log n)$ suffice, but only for very small crossover rates (≤ $1/n$)

More Theory on Crossover

- Sequence of follow-up works
  - Fischer&Wegener (GECCO 2004)
  - Storch&Wegener (TCS 2004)
  - Sudholt (GECCO 2005)
  - Jansen&Wegener (Disc. Appl. Math. 2005)

- …but all regard quite artificial problems
  - "It will take many major steps to prove rigorously that crossover is essential for typical applications." (Jansen&Wegener (2005))

- Insight: If it is so hard to find a single convincing problem where crossover provably helps, maybe crossover is not so important?

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 ☺
  [D., Happ, Klein (Gecco'08), D., Theile (Gecco'09), D.,Johannsen, Kötzing, Neumann, Theile (PPSN'10)]
  - 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"

- More recent works:
  - Sudholt (Gecco'12): Crossover can even help for the simple OneMax problem (constant factor improvement)
  - D., Doerr, Ebel (Gecco'13): $\sqrt{\log n}$ factor improvement for OneMax
    - working principle: crossover as repair mechanism (known from ES, first time in discrete optimization)

Example 3: Summary

Theory work on crossover:

- It was hard to find a single convincing example where crossover was provably helpful. Possibly, crossover is not so important, or it gives improvements too small to be visible with theory methods (e.g., constant factors improvements or lower order terms)
- The few examples where crossover works indicate that other principles than the building block hypothesis are more relevant.

The F-Words in Theory

- Besides (hopefully) short- or medium-term useful results, theory also ask and tries to answer questions that are

FUNDAMENTAL

- Besides being difficult, mathematical, tricky, full of negative surprises, theory can be

FUN

- I'll now show you how to bring the two together

A Fundamental Question

- How difficult is a problem for evolutionary methods?
- Since “evolutionary methods” is hard to define precisely (and we do theory), let us broaden the scope to black-box optimization.
- Black-box optimization: you do not have access to an explicit problem description, but all you can do is evaluate solution candidates.
  - evolutionary algorithms
  - ant colony optimization
  - local search, random search, …
- How difficult is a problem for black-box optimization = what is the performance of the best black-box algorithm for this problem?
  - black-box complexity (BBC) of the problem

Example: BBC of Needle Functions

- Needle functions: For all $z \in \{0,1\}^n$, let

$$f_z : \{0,1\}^n \to \{0,1\}; x \mapsto \begin{cases} 1, & x = z \\ 0, & x \neq z \end{cases}.$$

- How many fitness evaluations do you need to find the maximum of *any* of these functions?

- First answer: You can try all bit-strings one after the other.
After 2^n fitness evaluations, you surely found the optimum.
→ $BBC \leq 2^n$.

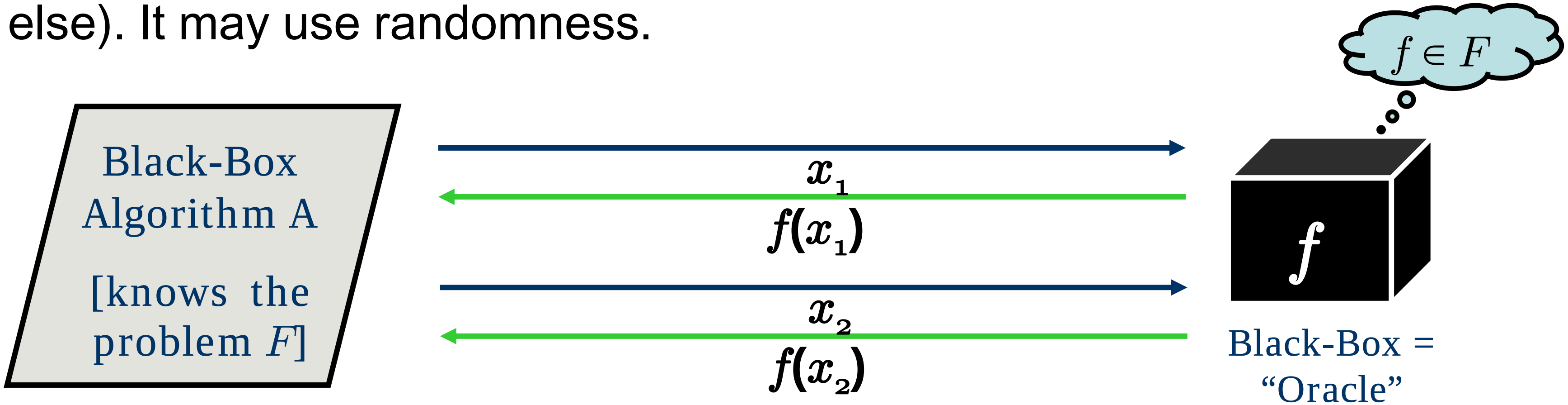
Definition of BBC

- This example made precise: For all $z \in \{0,1\}^n$, let

  $$f_z : \{0,1\}^n \to \{0,1\}; x \mapsto \begin{cases} 1, & x = z \\ 0, & x \neq z \end{cases}$$ "instance".

  Let $F := \{ f_z \mid z \in \{0,1\}^n \}$ "problem".

- A black-box algorithm A for F takes any $f_z \in F$ (blindly) as input. It may evaluate any $x \in \{0,1\}^n$ in a black-box fashion (it learns $f_z(x)$, but nothing else). It may use randomness.



Definition of BBC (2)

- This example made precise: For all $z \in \{0,1\}^n$, let

  $$f_z : \{0,1\}^n \to \{0,1\}; x \mapsto \begin{cases} 1, & x = z \\ 0, & x \neq z \end{cases}$$ "instance".

  Let $F := \{ f_z \mid z \in \{0,1\}^n \}$ "problem".

- A black-box algorithm A for F takes any $f_z \in F$ (blindly) as input and tries to find the optimum by evaluating search points.
  - $T(A, f_z) :=$ Expected number of evaluations until $OPT(f_z)$ is evaluated
  - $T(A, F) := \max_{f_z \in F} T(A, f_z)$
  - $BBC(F) := \min_A T(A, F)$ = "min number of fitness evaluation to solve F"
- $BBC(F) \leq 2^n$, because "ask all $x \in \{0,1\}^n$ in some fixed order" for any $f_z \in F$ needs at most 2^n fitness evaluations to query the optimum z of f_z

Lower Bounds

- Definition (reminder):
  - $T(A, f_z) :=$ Expected number of evaluations until $OPT(f_z)$ is evaluated
  - $T(A, F) := \max_{f_z \in F} T(A, f_z)$
  - $BBC(F) := \min_A T(A, F)$ = "min number of fitness evaluation to solve F"
- To prove a lower bound "$BBC(F) \geq xxx$", we need to show that *any black-box algorithm* A needs at least xxx fitness evaluations (for some f_z)
- For needle functions: $BBC(F) \geq (2^n + 1)/2 \approx 2^{n-1}$.
  - very informal argument: can't do better than trying random search points (without repetition)
  - Corollary: Any EA, GA, ACO algorithm, swarm intelligence method etc. needs at least $(2^n + 1)/2 \approx 2^{n-1}$ fitness evaluations to solve the Needle problem. Universal lower bound ☺

Lower Bound For Needle (Formal)

- Reminder: To prove a lower bound "$BBC(F) \geq xxx$", we need to show that any black-box algorithm needs at least xxx fitness evaluations (for some f_z)

- Theorem: For needle functions, we have $BBC(F) \geq (2^n + 1)/2$.

- Proof:
  - Let A be any black-box algorithm for needle functions.
  - Let $x_1, x_2, x_3, \ldots$ be the sequence of search points A evaluates. Note that this does not depend on f_z (except that we stop when $x_i = z$). Hence we may assume that A chooses (possibly randomly) an enumeration $x_1, x_2, x_3, \ldots$ of the search space $\{0,1\}^n$ and then evaluates $x_1, x_2, x_3, \ldots$ in that order until the optimum is found.
  - Some maths: For any random sequence $x_1, x_2, x_3, \ldots$ there is an f_z such that the expected position of z in the sequence is at least $(2^n + 1)/2$.

Example 2: OneMax Functions

- OneMax functions: For all $z \in \{0,1\}^n$, let

  $f_z : \{0,1\}^n \to \{0,1\}; x \mapsto eq(x,z) := |\{i \mid x_i = z_i\}|$ "# bits in which x, z agree"

  [hence $f_{(1,\dots,1)}$ is the classic OneMax function counting the 1s in the bit-string]

- What is the BBC of the OneMax functions?

- Upper bound 1: The (1+1) evolutionary algorithm optimizes any f_z in $en\ln(n)$ iterations → $BBC \le en\ln(n)$.

- Upper bound 2: You can learn the bits of z one after the other. E.g. if $f_z(1x_2 \dots x_n) \ge f_z(0x_2 \dots x_n)$, then $z_1 = 1$, else $z_1 = 0$. → $BBC \le n + 1$.

- Theorem [Erdős,Rényi '63]: $BBC(OneMax) = \Theta\left(\frac{n}{\log(n)}\right)$.

Example 2: OneMax Functions

- Theorem [Erdős,Rényi '63]: $BBC(OneMax) = \Theta\left(\frac{n}{\log(n)}\right)$.
  - There is a black-box algorithm finding the optimum z of any OneMax function $f_z : \{0,1\}^n \to \{0,1\}; x \mapsto eq(x,z) := |\{i \mid x_i = z_i\}|$ with only $2\, n/\log_2 n$ fitness evaluations.
  - There is no algorithm doing better than $n/\log_2 n$.

- Note: There are papers presenting faster algorithms for OneMax
→ these algorithms cannot work for all OneMax functions (because of the theorem above)
  - typically, these algorithms are designed for the "counting 1s" function only
  - in a sense, they derive their better performance by exploiting the fact that they know the optimal solution $(1, \dots, 1)$ already

Example 2: OneMax Functions

- Theorem [Erdős,Rényi '63]: $BBC(OneMax) = \Theta\left(\frac{n}{\log(n)}\right)$.

- ER'63-algorithm:
  - Evaluate $2\,n/\log_2 n$ random search points $x_1, x_2, \ldots$ and store their fitnesses $y_1, y_2, \ldots$
  - With high probability, there is only one f_z such that $f_z(x_i) = y_i$ for all x_i
  - Then z is the optimal solution ☺

- Comments:
  - This is an artificial algorithm and not useful for any real problem
  - But this is OK for now, because it tells us the black-box complexity of the OneMax problem.
  - We could use this as a trigger and ask ourselves if there are better EAs for OneMax (indeed, there are)

Fun: Mastermind

- Mastermind: 2-player game
  - *CodeMaker* hides a ~~4~~ n-digit ~~6~~ k-color code C.
  - *CodeBreaker* tries to guess it using few guesses
- Guess: Some color code G
- Answer:
  - Number of positions in which C and G agree ("black answer-pegs" [here: red])
  - ~~Number of additional code letters that occur in a wrong position ("white pegs")~~

Fun: Mastermind

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- Guess: Some color code G
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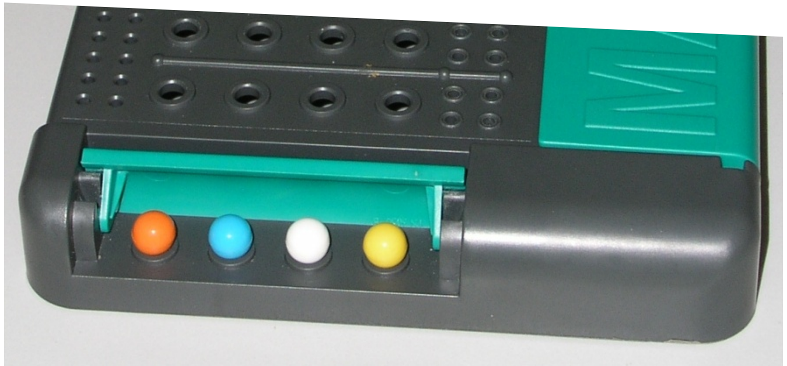
  - Number of positions in which C and G agree (“black answer-pegs” [here: red])
- Reminder: OneMax functions: For all $z \in \{0,1\}^n$, let $f_z : \{0,1\}^n \to \{0,1\}; x \mapsto eq(x,z) := |\{i \mid x_i = z_i\}|$ “# bits in which x, z agree”
- Observation: BBC(OneMax) ≙ n-digit 2-color Mastermind!
  - → You can win Mastermind with $2\,n/\log_2 n$ guesses

BBC and Population Size

- The OneMax functions have a surprisingly low BBC of only $2\,n/\log_2 n$.
  - Most evolutionary algorithms need at least $n\ln(n)$ fitness evaluations.
- Question: Can this discrepancy be explained by the fact that the ER'63 black-box algorithm stores $2\,n/\log_2 n$ search points? Is the black-box complexity larger when we restrict the memory to some $k < 2\,n/\log_2 n$.
  - Note: Use restricted BBCs to gain fundamental insight about EA parameters, here the population size
- Conjecture (Droste, Jansen, Wegener (2006)): For $k = 1$, the memory restricted BBC is of order $n\log n$.
- Theorem (Doerr&Winzen (2012)): No, even with memory $k = 1$, the BBC remains at a low $cn/\log n$, where c is some (unknown) constant.

Fun Fact: Memory-1 BBC(OneMax) = Mastermind with Only Two Rows

- Precise rules:
  - We start the game with an empty board
  - If there is an empty row, CodeBreaker can enter a guess, which will be answered by CodeMaker
  - If there is no empty row, CodeBreaker must empty one of the two rows and *forget the content*.



- Observation: Black-box algorithms with memory restriction $k = 1$ exactly correspond to strategies for Mastermind with two rows
- **Theorem: CodeBreaker can find the secret code with $O(n / \log n)$ guesses even when there are only two rows.**
- PS: There is a BBC paper at PPSN'14 (by Badkobeh, Lehre, Sudholt), tomorrow first session

Final Summary

- Theory (strict definition): Precise results proven with mathematical rigor.
- Complements well with experiments
  - Theory: safest possible assertion, reader can check the proof, "for all" statements, many problems too complicated to prove exact bounds or something at all
  - Experiments: more error-prone, less reproducibility, finite number of tests, exact numbers, real-world examples
- Achievements:
  - debunk misbeliefs
  - give advice in algorithm design
  - understand working principles of EA

Hvala!

Thanks!

- PS: We'll put the slides on the PPSN page, sorry for being late.