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LAMDA
Learning And Mining from Data
<http://www.lamda.nju.edu.cn>



Why Do We Need Theoretical Research of Evolutionary Algorithms?

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Theory

“A theory is a rational type of abstract thinking about a phenomenon, or the results of such thinking.”
From Wikipedia

Notions of Theory in Evolutionary Computation

- Experimentally guided theory: Design an experiment to empirically study a question
- Descriptive theory: Describe/measure/quantify observations
- “Theory”: Unproven claims, e.g., building block hypothesis
[Goldberg, 1989] Critiqued, even wrong [Reeves and Rowe, 2002]
- Theory: Mathematically proven results What we mean here

Schema theorem



Schema theorem [Holland, 1975]

- To explain how the population of genetic algorithms changes in steps

Study the change of $m(H, t)$ of Simple Genetic Algorithm

$$E[m(H, t + 1)] \geq m(H, t) \cdot \frac{\bar{f}_H}{\bar{f}} \cdot \left(1 - \left(p_c \cdot \frac{d(H)}{n-1}\right)\right) \cdot (1 - p_m)^{o(H)}$$

- Schema H is a template with “#” = “any”, which defines a subspace
- $m(H, t)$: number of individuals belonging to schema H in the t -th population

01#1#

Schema theorem



Schema theorem [Holland, 1975]

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*Average fitness of individuals
belonging to H in the pop.*

selection

*Average fitness of
individuals in the pop.*

*Prob. of not disrupting H
by one-point crossover*

recombination

*Prob. of not disrupting H
by bit-wise mutation*

mutation

Schema theorem



Schema theorem [Holland, 1975]

- To explain how the population of genetic algorithms changes in steps

Study the change of $m(H, t)$ of Simple Genetic Algorithm

$$E[m(H, t + 1)] \geq m(H, t) \cdot \frac{\overline{f_H}}{\bar{f}} \cdot \left(1 - \left(p_c \cdot \frac{d(H)}{n-1}\right)\right) \cdot (1 - p_m)^{o(H)}$$

Low-order and short schema of above-average fitness is more likely to survive

Limitation: ignoring the constructive effect of the operators; explain the local behaviors only

No free lunch theorem



No free lunch theorem [Wolpert and Macready, TEVC 1997]

- To understand the relationship between how well a black-box optimization algorithm performs and the optimization problem on which it is run

Expected Performance of an algorithm \mathcal{A} iterated m times on a cost function f

$$\sum_f \left[\sum_{d_m^y} \Phi(d_m^y) P(d_m^y \mid f, m, \mathcal{A}_1) \right] = \sum_f \left[\sum_{d_m^y} \Phi(d_m^y) P(d_m^y \mid f, m, \mathcal{A}_2) \right]$$

Diagram showing two arrows pointing from the boxed expressions to the text "Expected Performance of an algorithm \mathcal{A} iterated m times on a cost function f ".

No free lunch theorem



No free lunch theorem [Wolpert and Macready, TEVC 1997]

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$$\sum_f \sum_{d_m^y} \Phi(d_m^y) P(d_m^y \mid f, m, \mathcal{A}_1) = \sum_f \sum_{d_m^y} \Phi(d_m^y) P(d_m^y \mid f, m, \mathcal{A}_2)$$



Any two algorithms are equally good across all problems over the uniform distribution

Also hold for supervised learning algorithms [Wolpert, Neural Computation 1996]

Limitation: NOT a uniform prior in practice

What theory now we focus on?

Goals of design and analysis of algorithms

- **Correctness** *“Is the solution output by the algorithm always correct?”*
- **Computational complexity** *“How many computational resources are required?”*

For evolutionary algorithms,

- **Convergence** *“Does the EA find a global optimum with prob. 1 as #generations goes to infinity?”*
- **Running time complexity** *“How long does it take to find an (approximate) optimum?”*

Convergence

Does an EA converge to a global optimum?

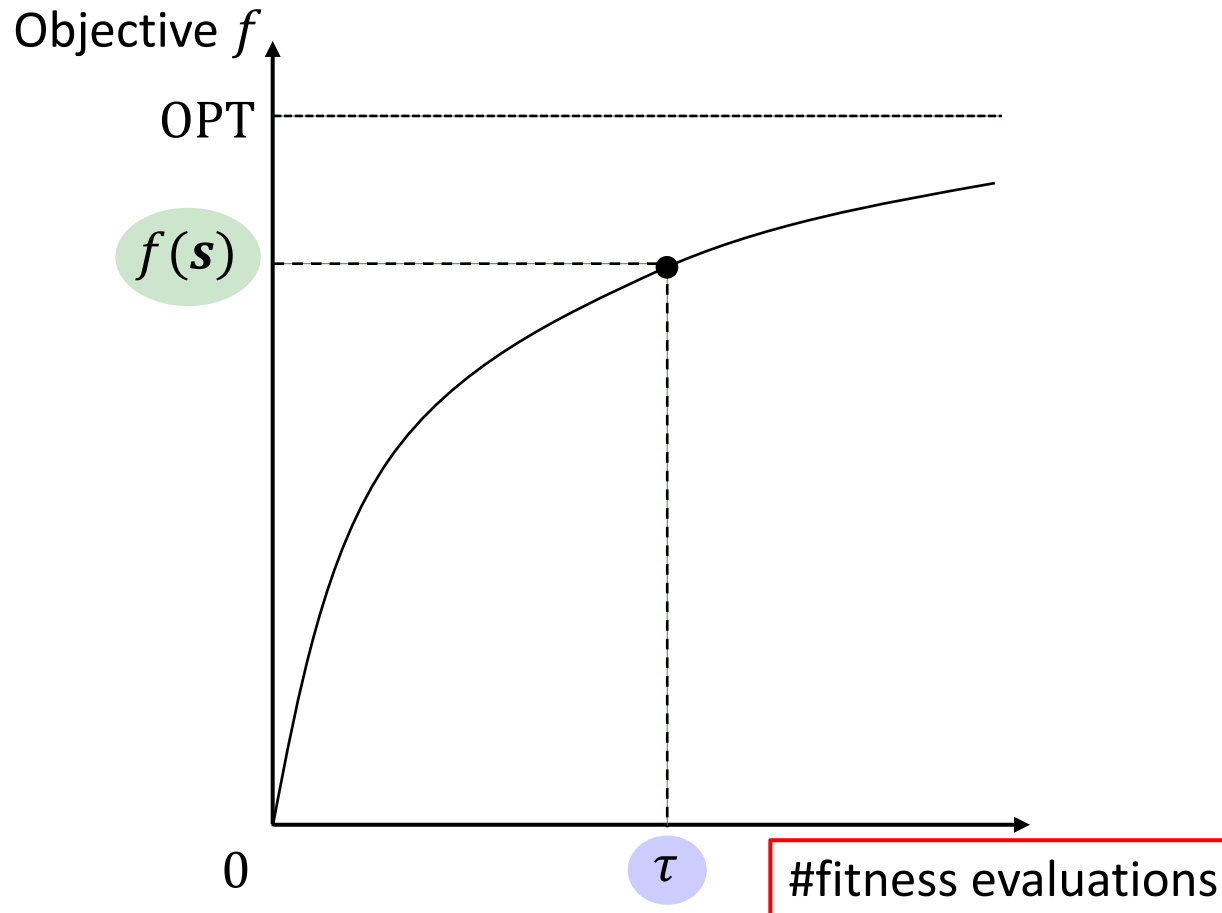
$$\lim_{t \rightarrow +\infty} P(\xi_t \in \mathcal{X}^*) = 1$$

Sufficient conditions [Rudolph, 1998]:

- Use global reproduction operators (a positive probability to reach any point)
- Preserve the best found solution (elitism)

But life is limited! How fast does it converge?

Running time complexity



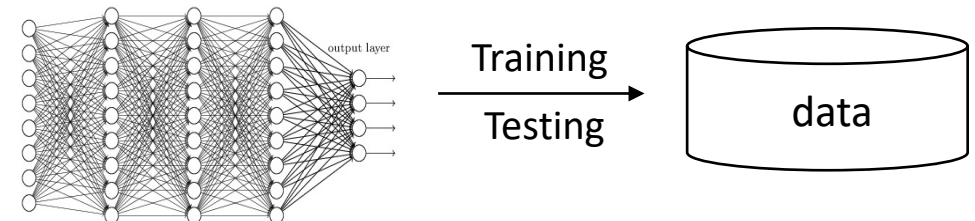
What we concern:

- $E[\tau]$
- $P(\tau \leq T)$

Running time τ :

#fitness evaluations until finding desired solutions for the first time

the process with the highest cost of EA
e.g., model evaluation



Running time analysis

Fitness Level
[Wegener, 2000]



I. Wegener (1950-2008)
TU Dortmund, Germany
Pioneer of EC Theory

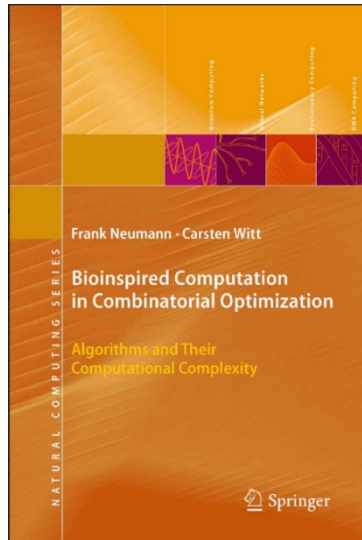
Drift Analysis
[He & Yao, AIJ'01]



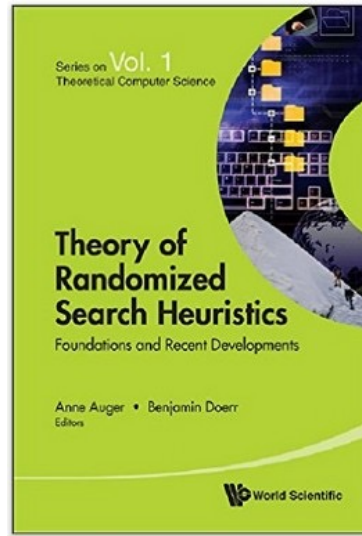
X. Yao
SUSTech, China
IEEE Frank Rosenblatt Award

Switch Analysis
[Yu, Qian & Zhou, TEVC'15]

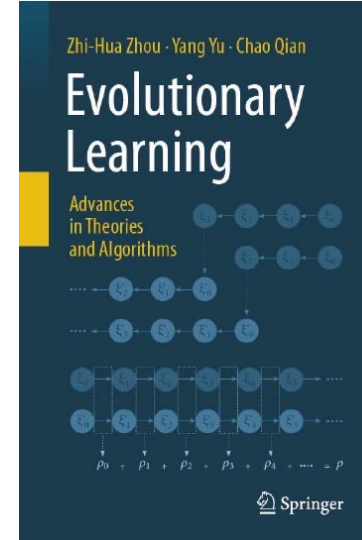
Stefan Droste, Thomas Jansen, Ingo Wegener:
A Rigorous Complexity Analysis of the $(1 + 1)$ Evolutionary Algorithm for Separable Functions with Boolean Inputs.
Evolutionary Computation 6(2): 185-196 (1998)



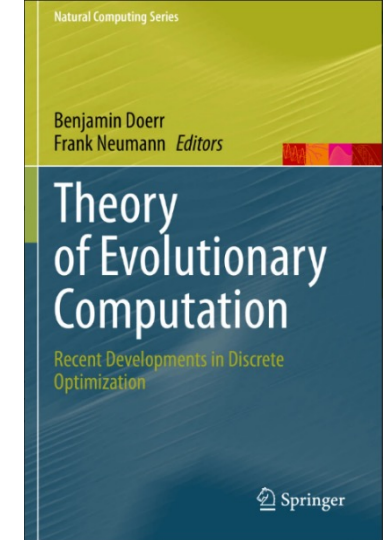
[Neumann and Witt, 2010]



[Auger and Doerr, 2011]



[Zhou, Yu and Qian, 2019]



[Doerr and Neumann, 2020]

How running time analysis can help us?

- Help understand behaviors of EAs
- Guide the design of EAs
- Generate EAs with theoretical guarantees

Example illustration: Help understand behaviors of EAs

Mutation and **recombination** are two characterizing features of EAs

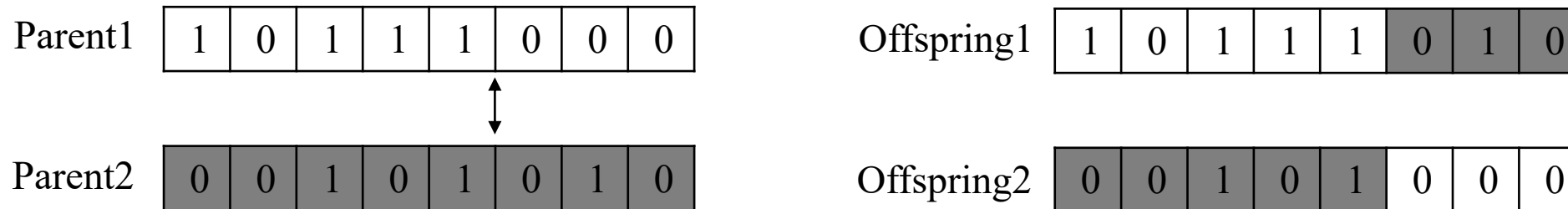
Example of **mutation**



simulates the gene altering of a chromosome in biological mutation

Example of **recombination**

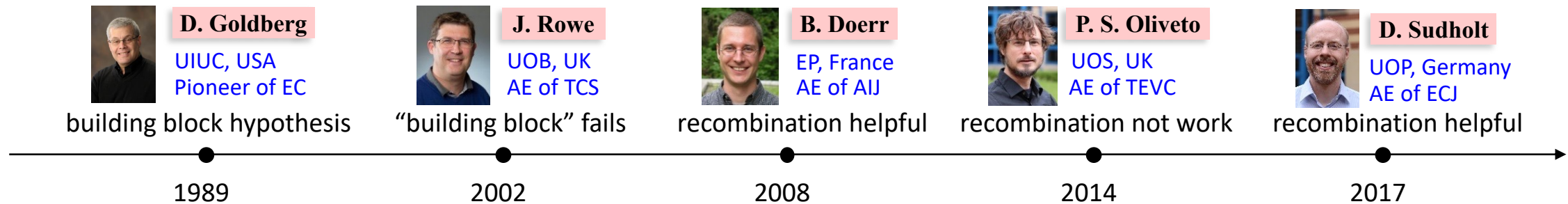
More complicated



simulates the chromosome exchange phenomena in zoogamy reproductions

Example illustration: Help understand behaviors of EAs

Most theoretical studies focused on EAs with mutation, while **only a few included recombination**, which is difficult to be analyzed due to the irregular behavior



Mainly focused on single-objective optimization

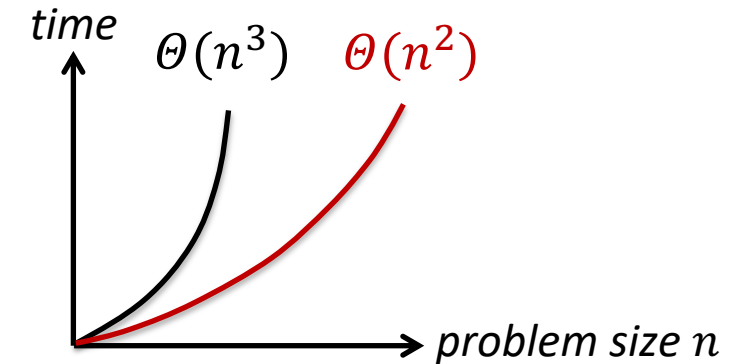
How about the influence of recombination for **multi-objective optimization**?

- Important applications of EAs
- More complex than single-objective optimization

Example illustration: Help understand behaviors of EAs

Theorem: For GSEMO solving the LOTZ problem

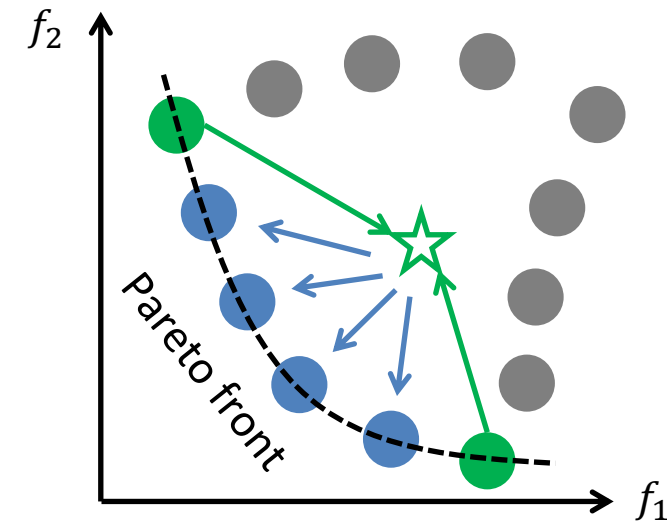
Expected running time $\Theta(n^3)$ recombination \longrightarrow $\Theta(n^2)$



Our findings:

Recombination can accelerate the filling of the Pareto front by recombining diverse Pareto optimal solutions

Unique to multi-objective optimization



Example illustration: Guide the design of EAs

Pareto dominance based: NSGA-II, SPEA-II, ...



K. Deb, A. Pratap, S. Agarwal and T. Meyarivan. A fast and elitist multiobjective genetic algorithm: NSGA-II. *IEEE Transactions on Evolutionary Computation*, 2002. (Google scholar citations: 45628)

Performance indicator based: SMS-EMOA , HyPE,



N. Beume, B. Naujoks and M. Emmerich. SMS-EMOA: Multiobjective selection based on dominated hypervolume. *European Journal of Operational Research*, 2007. (Google scholar citations: 1909)

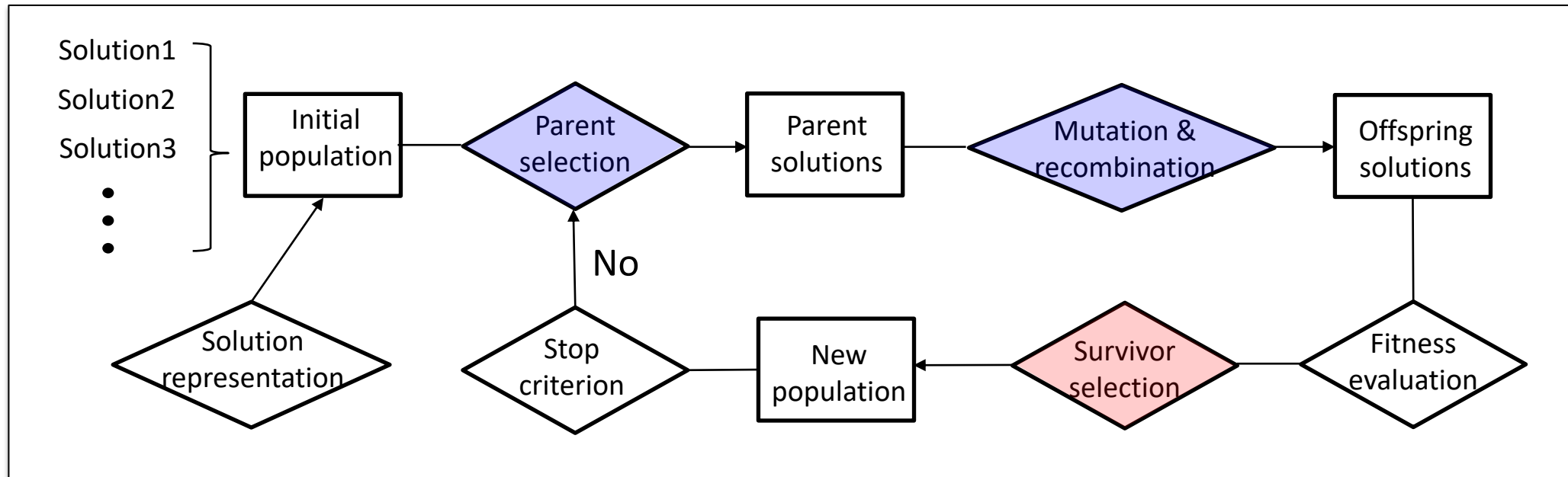
Decomposition based: MOEA/D,



Q. Zhang and H. Li. MOEA/D: A multiobjective evolutionary algorithm based on decomposition. *IEEE Transactions on Evolutionary Computation*, 2007. (Google scholar citations: 7515)

Example illustration: Guide the design of EAs

Two key components of MOEAs: **solution generation** and **population update**

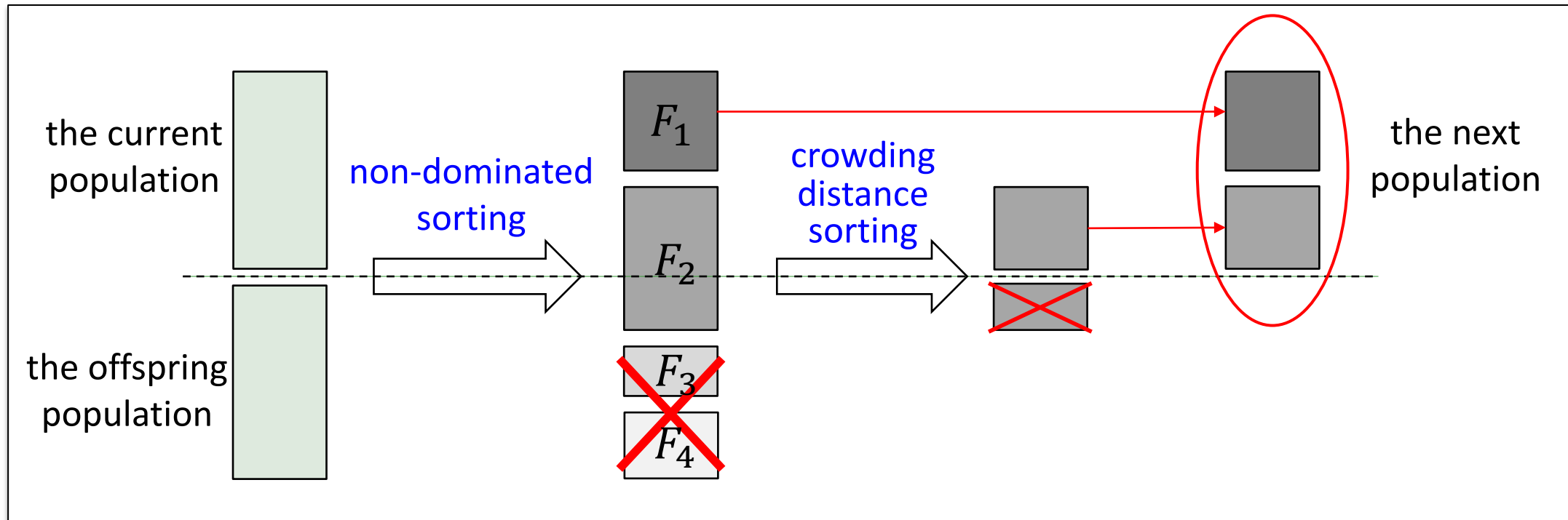


In the area of evolutionary multi-objective optimization, the research focus is mainly on population update

Example illustration: Guide the design of EAs

Population Update of NSGA-II:

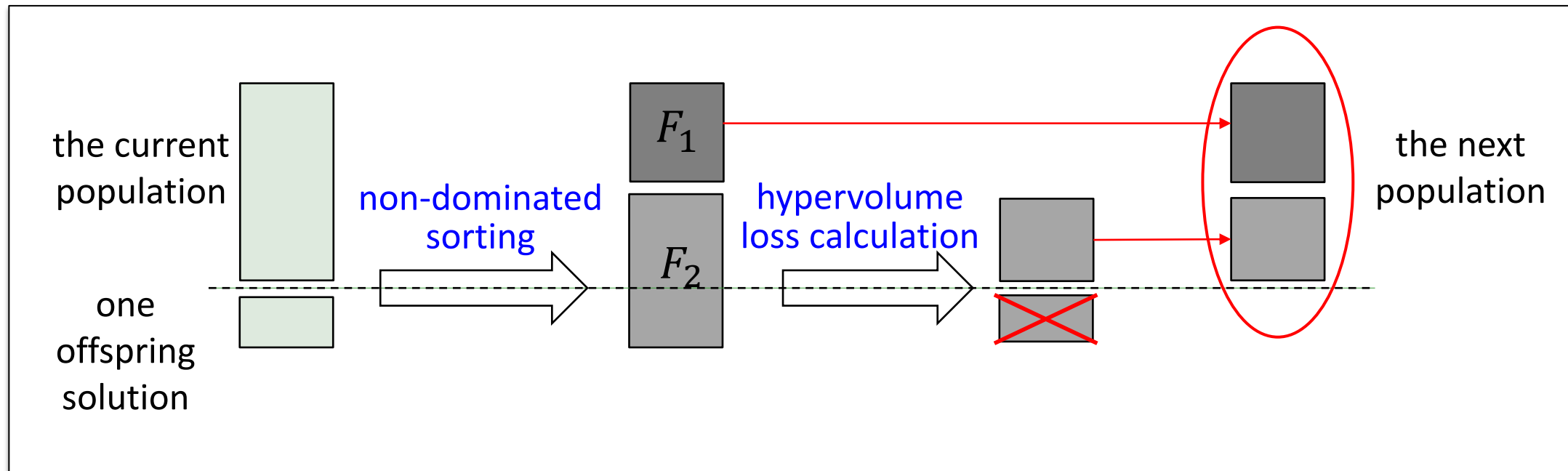
Use **non-dominated sorting** and **crowding distance sorting** to rank the solutions, and **delete the worst ones**



Example illustration: Guide the design of EAs

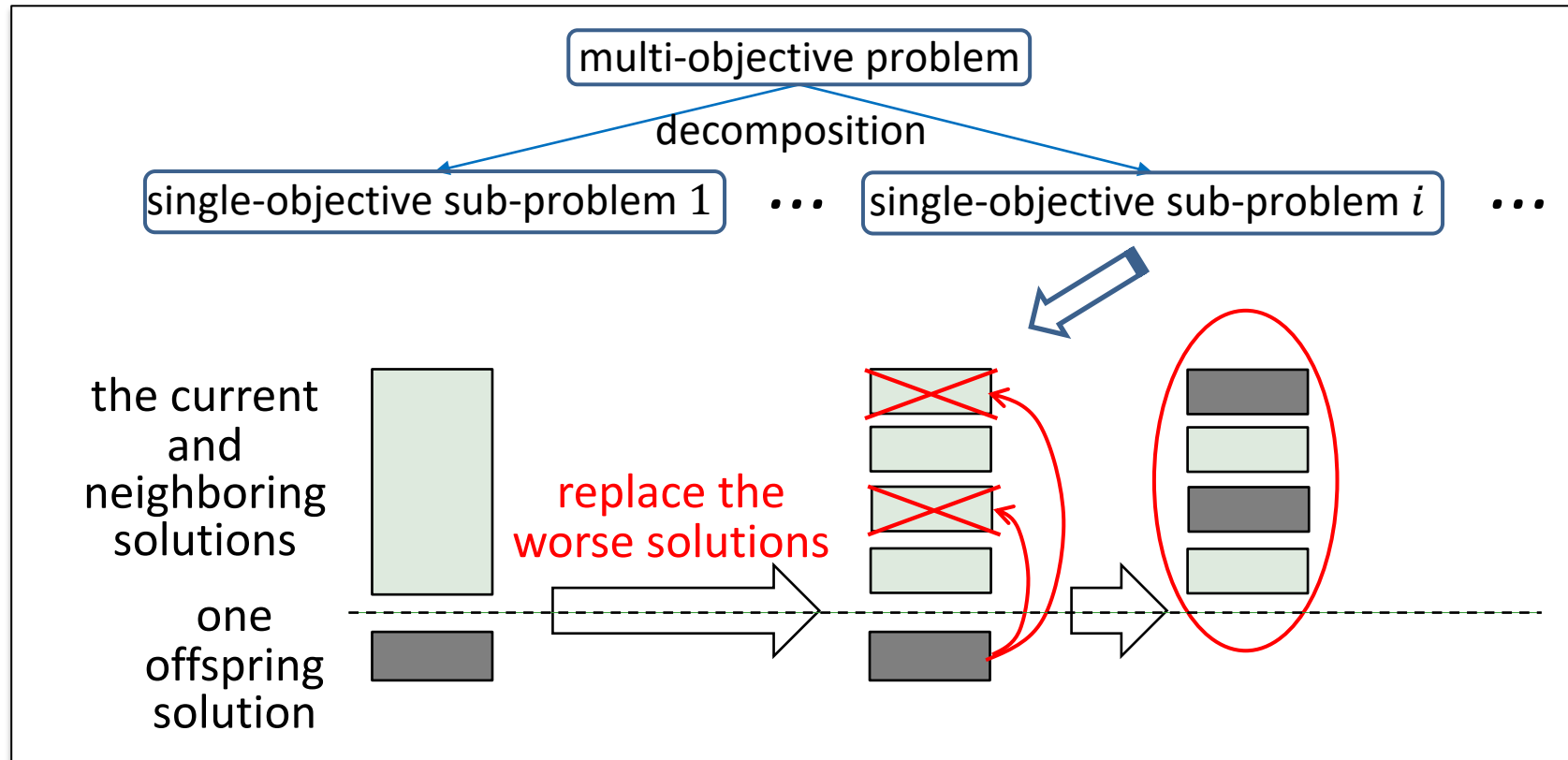
Population Update of SMS-EMOA:

Use **non-dominated sorting** and **quality indicators (e.g., hypervolume)** to rank the solutions, and **delete the worst solution**



Example illustration: Guide the design of EAs

Population Update of MOEA/D:



Example illustration: Guide the design of EAs

The prominent feature in population update of MOEAs: Greedy and deterministic

- the next-generation population is formed by selecting the best-ranked solutions



K. Deb

*“One common aspect of these **first-generation multi-objective algorithms** is that **they did not use any elite-preservation operator**, thereby compromising the **performance** and was also contrary to Rudolph’s asymptotic convergence proof which required the preservation of elites from one generation to the next.”*

An Interview with Kalyanmoy Deb 2022 ACM Fellow

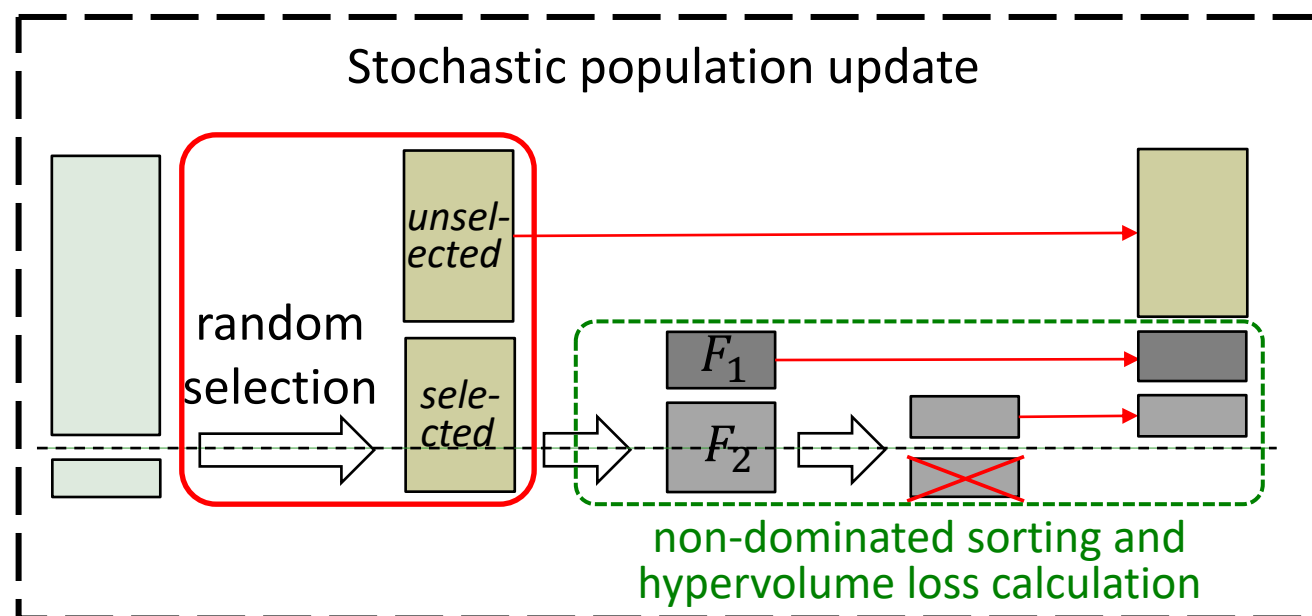
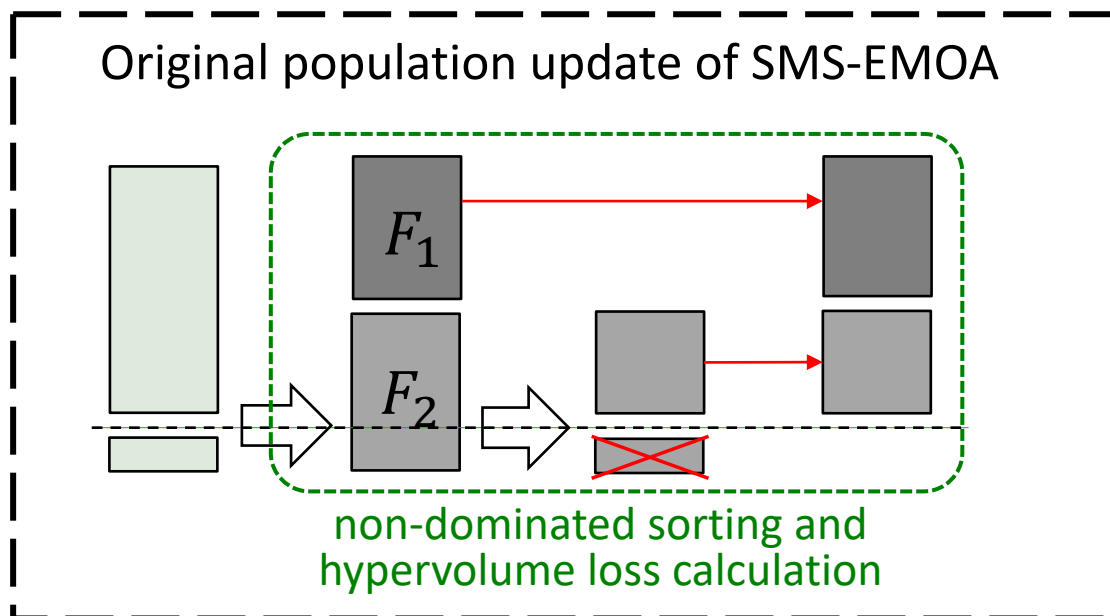
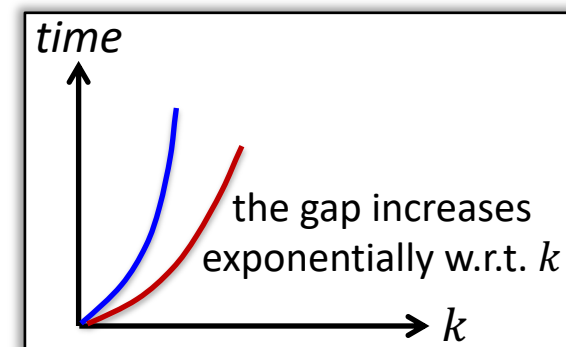
Is deterministic population update always better?

NO!

Example illustration: Guide the design of EAs

Theorem: For SMS-EMOA solving the OneJumpZeroJump problem

Expected running time $\Omega(n^k)$ Stochastic
 $\xrightarrow[\text{exponentially faster}]{\text{accelerate by } 2^{k/4}/\mu^2}$ $O(\mu n^k \cdot \min\{1, \mu/2^{k/4}\})$



Example illustration: Guide the design of EAs

The OneJumpZeroJump problem:

$$f_1(\mathbf{x}) = \begin{cases} k + |\mathbf{x}|_1, & \text{if } |\mathbf{x}|_1 \leq n - k \text{ or } \mathbf{x} = 1^n \\ n - |\mathbf{x}|_1, & \text{else} \end{cases}$$

$$f_2(\mathbf{x}) = \begin{cases} k + |\mathbf{x}|_0, & \text{if } |\mathbf{x}|_0 \leq n - k \text{ or } \mathbf{x} = 0^n \\ n - |\mathbf{x}|_0, & \text{else} \end{cases}$$

Characterize a class of problems where some adjacent Pareto optimal solutions in the objective space locate far away in the decision space

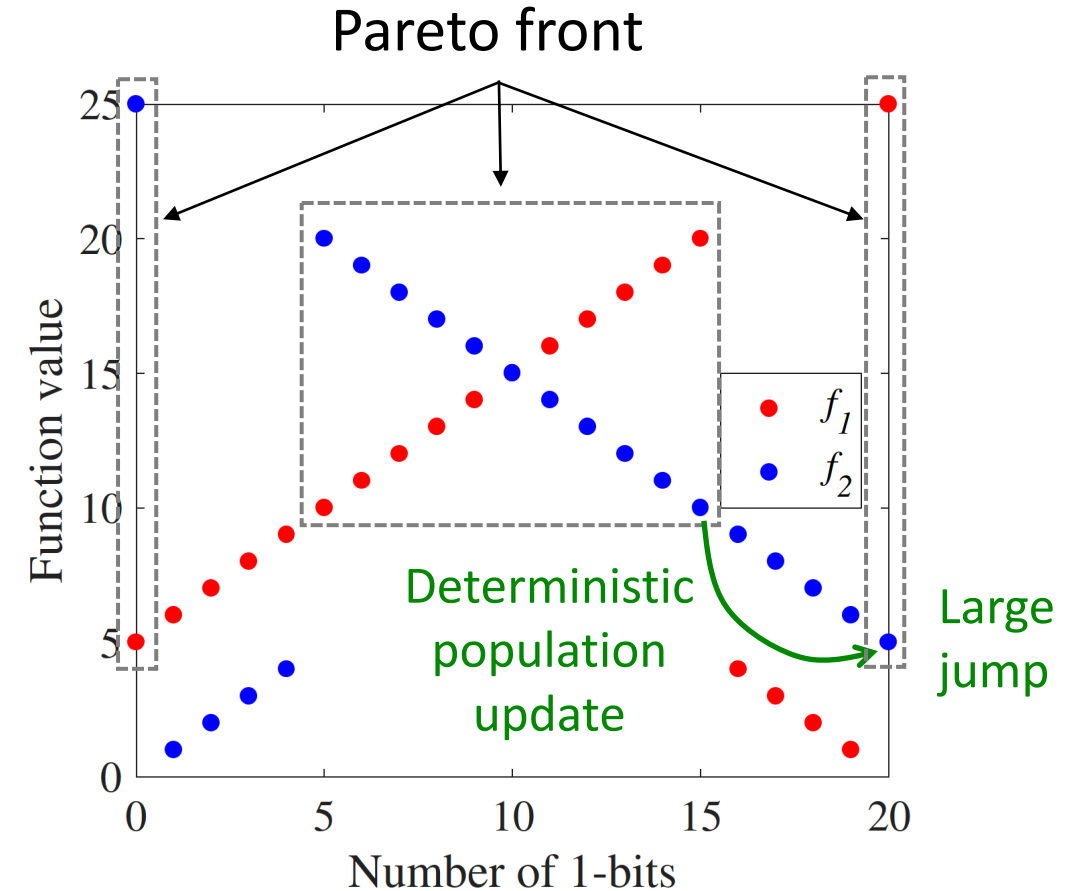


Illustration of function values
when $n = 20$ and $k = 5$

Example illustration: Guide the design of EAs

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$$f_1(\mathbf{x}) = \begin{cases} k + |\mathbf{x}|_1, & \text{if } |\mathbf{x}|_1 \leq n - k \text{ or } \mathbf{x} = 1^n \\ n - |\mathbf{x}|_1, & \text{else} \end{cases}$$

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Characterize a class of problems where some adjacent Pareto optimal solutions in the objective space locate far away in the decision space

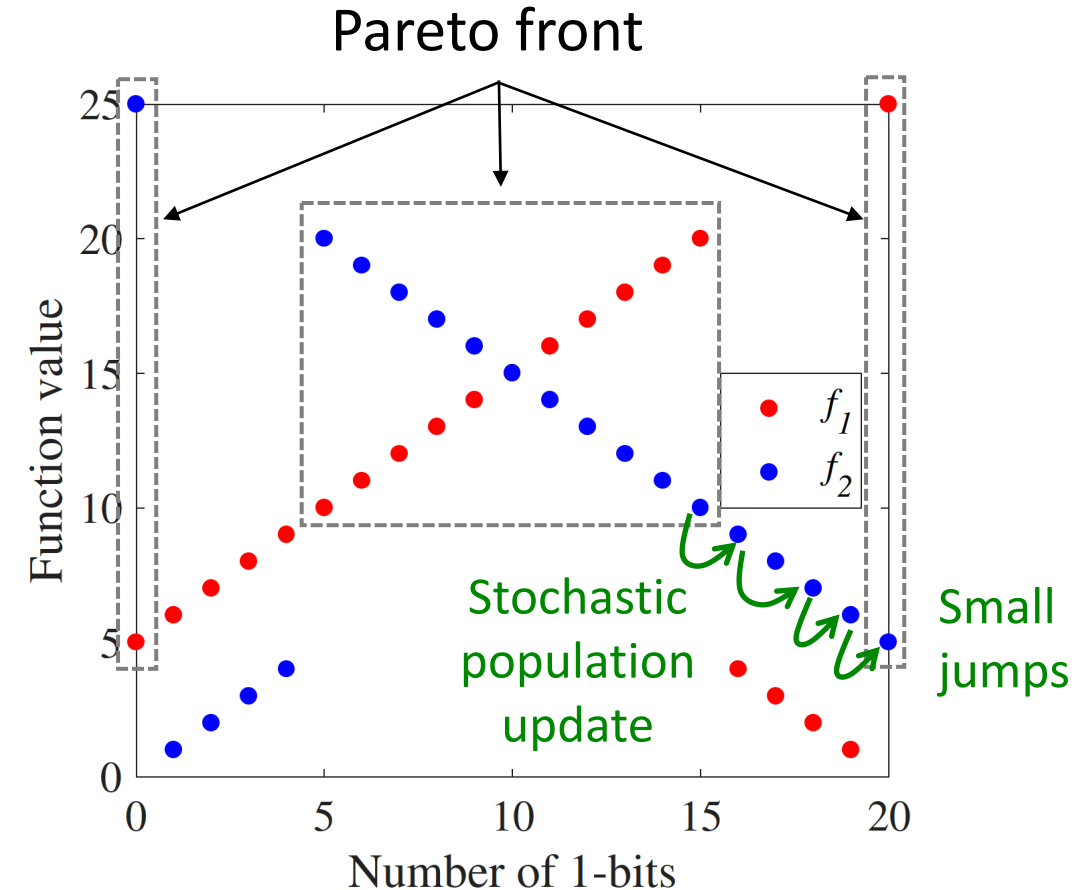


Illustration of function values
when $n = 20$ and $k = 5$

Example illustration: Guide the design of EAs

Introducing randomness into population update can make MOEAs go across inferior regions between different Pareto optimal solutions more easily

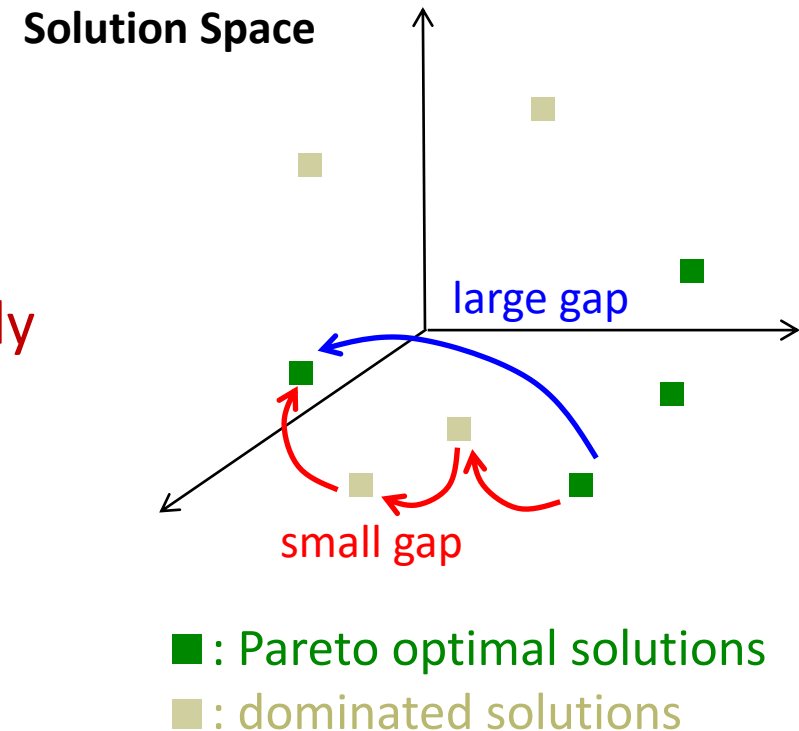
➤ Deterministic

- prefers non-dominated solutions
- if the points in the Pareto front are far away in the solution space, easy to get trapped

➤ Stochastic

May hold more generally

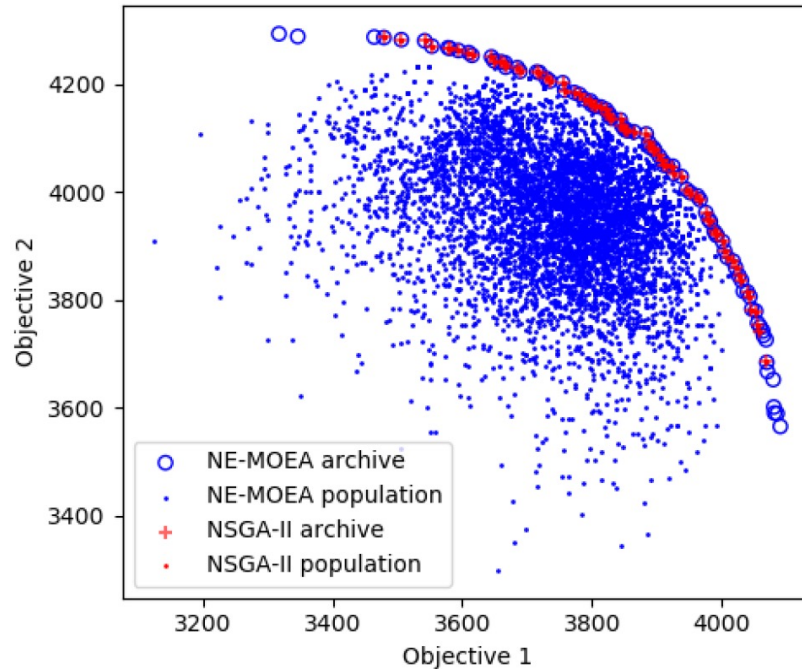
- allows dominated solutions to participate in the evolutionary process
- may follow an easier path in the solution space to find points in the Pareto front



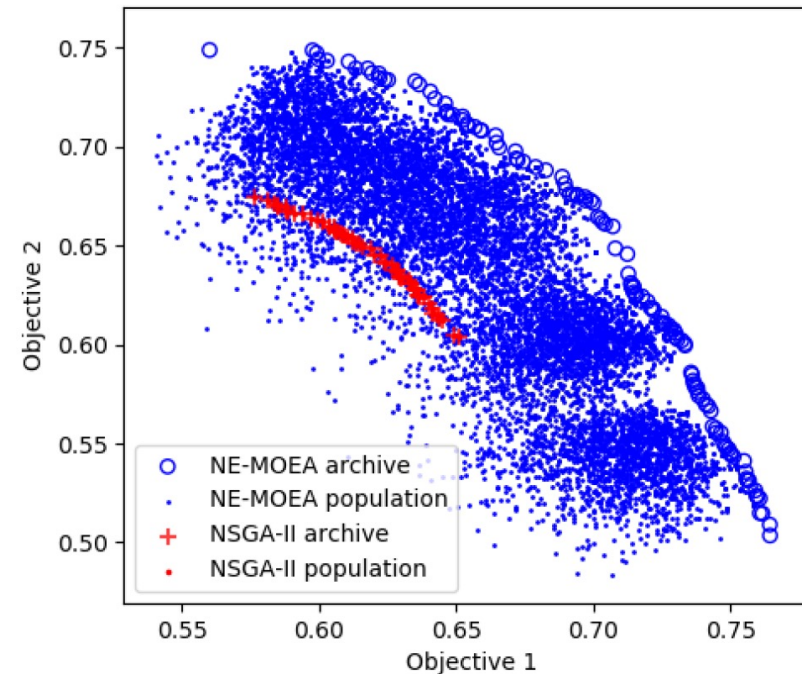
Example illustration: Guide the design of EAs

Encourage the exploration of developing new MOEAs in the area

For example [Liang, Li and Lehre, arXiv'23]: **NSGA-II** vs. **Non-elitist MOEA (NE-MOEA)**



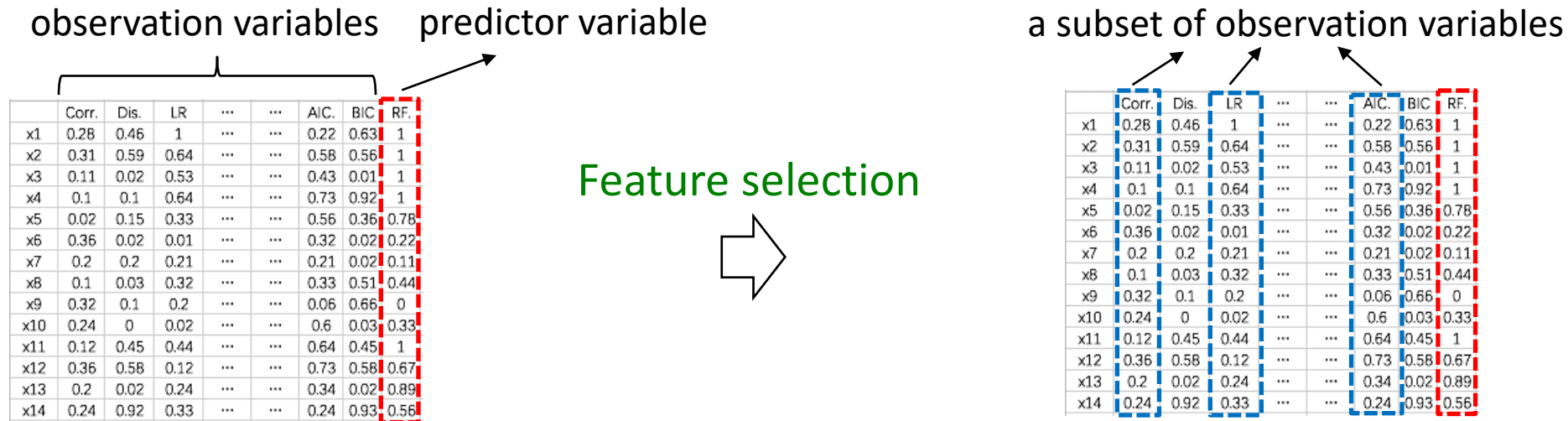
On knapsack with 100 items



On NK-Landscape with $n = 200$ and $k = 10$

Example illustration: Generate EAs with theoretical guarantees

There are many applications of selecting a good subset from a ground set

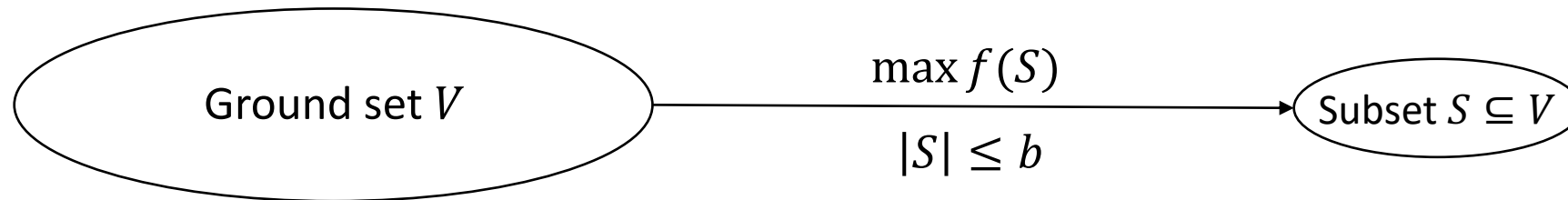
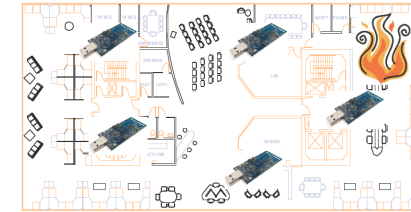
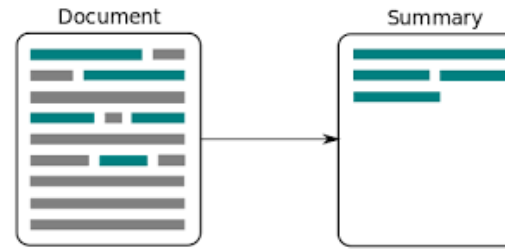


Example illustration: Generate EAs with theoretical guarantees

There are many applications of **selecting a good subset from a ground set**

Sparse regression Influence maximization Document summarization Sensor placement

	Corr	Dis	LR	AIC	BIC	R ²
x1	0.28	0.46	1	0.22	0.6	1
x2	0.31	0.59	0.64	0.58	0.5	1
x3	0.11	0.02	0.53	0.43	0.04	1
x4	0.1	0.1	0.64	0.73	0.9	1
x5	0.02	0.15	0.33	0.56	0.3	0.78
x6	0.36	0.02	0.01	0.32	0.0	0.22
x7	0.2	0.2	0.21	0.21	0.02	0.11
x8	0.1	0.03	0.32	0.33	0.5	0.44
x9	0.32	0.1	0.2	0.06	0.6	0
x10	0.24	0	0.02	0.6	0.0	0.33
x11	0.12	0.45	0.44	0.64	0.4	1
x12	0.36	0.58	0.12	0.73	0.59	0.57
x13	0.2	0.02	0.24	0.34	0.02	0.89
x14	0.24	0.92	0.33	0.24	0.5	0.56



Subset Selection: Given all items $V = \{v_1, \dots, v_n\}$, an objective function $f: 2^V \rightarrow \mathbb{R}$ and a budget b , to select a subset $S \subseteq V$ such that

$$\max_{S \subseteq V} f(S) \quad \text{s.t.} \quad |S| \leq b \quad \text{NP-hard}$$

Example illustration: Generate EAs with theoretical guarantees

Introduce the Pareto optimization algorithm for subset selection (POSS)

$$\begin{array}{ccc} \text{Constrained} & \xrightarrow{\text{Transformation}} & \text{Bi-objective} \\ \max_{S \subseteq V} f(S) \quad \text{s.t.} \quad |S| \leq b & & \min_{S \subseteq V} (-f(S), |S|) \end{array}$$

Algorithm 14.2 POSS Algorithm

Input: $V = \{v_1, v_2, \dots, v_n\}$; objective function $f : \{0, 1\}^n \rightarrow \mathbb{R}$; budget $b \in [n]$

Parameter: number T of iterations; isolation function $I : \{0, 1\}^n \rightarrow \mathbb{R}$

Output: solution $s \in \{0, 1\}^n$ with $|s|_1 \leq b$

Process:

```

1: let  $s = 0^n$  and  $P = \{s\}$ ;
2: let  $t = 0$ ;
3: while  $t < T$  do
4:   select a solution  $s$  from  $P$  uniformly at random;
5:   apply bit-wise mutation on  $s$  to generate  $s'$ ;
6:   if  $\nexists z \in P$  such that  $I(z) = I(s')$  and  $z \succ s'$  then
7:      $Q = \{z \in P \mid I(z) = I(s') \wedge s' \succeq z\}$ ;
8:      $P = (P \setminus Q) \cup \{s'\}$ 
9:   end if
10:   $t = t + 1$ 
11: end while
12: return  $\arg \max_{s \in P, |s|_1 \leq b} f_1(s)$ 
  
```

Initialization: put the special solution 0^n into the population P

Reproduction: pick a solution randomly from P , and mutate it to generate a new one

Evaluation & selection: if the new solution is not dominated, put it into P and delete bad solutions

MOEA

Output: select the best feasible solution

Example illustration: Generate EAs with theoretical guarantees

POSS can achieve the optimal polynomial-time approximation guarantee

Theorem. For subset selection with monotone objective functions, POSS with $\mathbb{E}[T] \leq 2eb^2n$ and $I(\cdot) = 0$, i.e., a constant function, can find a solution s with $|s|_1 \leq b$ and $f(s) \geq (1 - e^{-\gamma_{\min}}) \cdot \text{OPT}$, where $\gamma_{\min} = \min_{s: |s|_1=b-1} \gamma_{s,b}$.

$\forall S \subseteq T \subseteq V: f(S) \leq f(T)$

#iterations

Proved to be the optimal polynomial-time approximation [Harshaw et al., ICML'19]

Experiments

Good reported results

Data set 1	✓
Data set 2	✓
Data set 3	✓
Data set 4	✓
Data set 5	✓

Performance on other data?

Data set 6	?
Data set 7	?
Data set 8	?
Data set 9	?
Data set 10	?

Guaranteed

Safe!

Remark: Theoretical guarantee implies worst-case performance

Example illustration: Generate EAs with theoretical guarantees

[Chao Qian. Can Evolutionary Clustering Have Theoretical Guarantees?
IEEE Transactions on Evolutionary Computation, in press]

Yes!

Theorem 1. For k -center clustering, the GSEMO achieves a 2-approximation ratio in polynomial running time.

Theorem 2. For discrete k -median clustering, the GSEMO achieves a $\frac{1}{1-\epsilon} \left(3 + \frac{2}{p}\right)$ -approximation ratio in polynomial running time.

Theorem 3. For k -means clustering, the GSEMO achieves a $\frac{1+\epsilon}{(1-\epsilon)^2} \left(3 + \frac{2}{p}\right)^2$ -approximation ratio in polynomial running time.


Theorem 4. For β -fair discrete k -median clustering, the GSEMO achieves a $(84, 7)$ -bicriteria approximation ratio in polynomial running time.

Example illustration: Generate EAs with theoretical guarantees

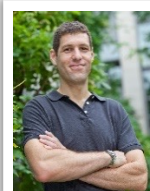
Approximation ratio under noise

Theorem. For subset selection under multiplicative noise with the assumption Eq. (17.29), with probability at least $(1/2)(1 - (12nb^2 \log 2b)/l^{2\delta})$, PONSS with $\theta \geq \epsilon$ and $T = 2e \ln b^2 \log 2b$ finds a solution s with $|s|_1 \leq b$ and $f(s) \geq \frac{1-\epsilon}{1+\epsilon} (1 - e^{-\gamma}) \cdot \text{OPT}$.

PONSS $\frac{f(S)}{\text{OPT}} \geq \frac{1-\epsilon}{1+\epsilon} (1 - e^{-\gamma})$ Significantly better



Greedy [Horel and Singer, NIPS'16]

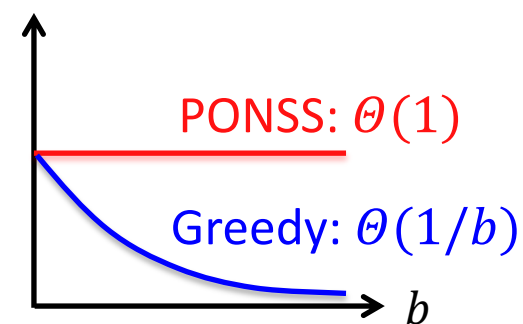


Y. Singer

Gordon McKay
Prof., Harvard

$$\frac{f(S)}{\text{OPT}} \geq \frac{1}{1 + \frac{2\epsilon b}{(1-\epsilon)\gamma}} \left(1 - \left(\frac{1-\epsilon}{1+\epsilon} \right)^b e^{-\gamma} \right)$$

approximation ratio



constant γ and ϵ

EAs achieve better approximation guarantees than conventional algorithms

How running time analysis can help us?

- Help understand behaviors of EAs
- Guide the design of EAs
- Generate EAs with theoretical guarantees

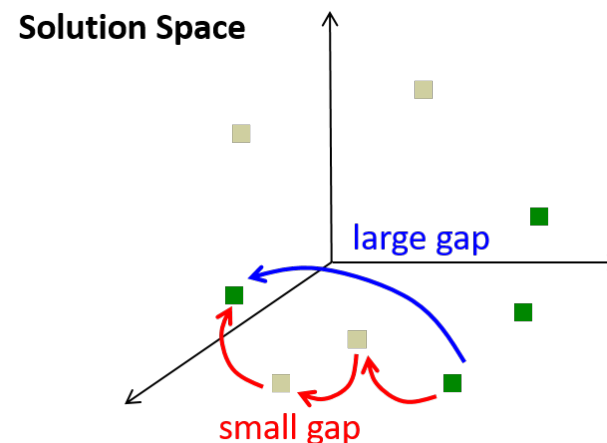
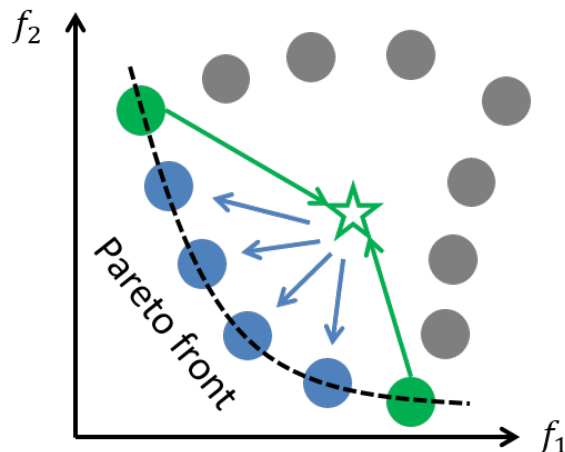
Why do theory?

Estimate the running time complexity by experiments



Why do theory? Because

- Absolute guarantee about the correctness
- Proofs (automatically) give insight in how things work



■ : Pareto optimal solutions
■ : dominated solutions

Why do theory?

Estimate the running time complexity by experiments



Why do theory? Because

- Absolute guarantee about the correctness
- Proofs (automatically) give insight in how things work
- Many results (e.g., on an algorithm/problem class) can be obtained only by theory

Theorem. For subset selection with monotone objective functions POSS with $\mathbb{E}[T] \leq 2eb^2n$ and $I(\cdot) = 0$, i.e., a constant function, can find a solution s with $|s|_1 \leq b$ and $f(s) \geq (1 - e^{-\gamma_{\min}}) \cdot \text{OPT}$, where $\gamma_{\min} = \min_{s: |s|_1=b-1} \gamma_{s,b}$.

Hold for any application of subset selection, any problem size n , and any budget b

Limitations of theoretical research

Limitations: Very difficult to obtain!

Theory and experiments are complementary

- Difficult to obtain theory, **do experiments**
- Even there is theory, experiments are still needed

E.g., we derive the expected running time $O(n^2)$ by theoretical analysis

But how about the coefficient? **Do experiments**

Limitations of theoretical research

Limitations: Very difficult to obtain!

Theory and experiments are complementary

- Difficult to obtain theory, do experiments
- Even there is theory, experiments are still needed

E.g., POSS can achieve the optimal polynomial-time approximation guarantee

Theorem. For subset selection with monotone objective functions, POSS with $\mathbb{E}[T] \leq 2eb^2n$ and $I(\cdot) = 0$, i.e., a constant function, can find a solution s with $|s|_1 \leq b$ and $f(s) \geq (1 - e^{-\gamma_{\min}}) \cdot \text{OPT}$, where $\gamma_{\min} = \min_{s: |s|_1=b-1} \gamma_{s,b}$.

Not bad in the worst case

Limitations of theoretical research

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Not bad in the worst case

Do experiments

Data set	OPT	POSS	FR	FoBa	OMP	RFE	MCP
housing	.7437±.0297	.7437±.0297	.7429±.0300●	.7423±.0301●	.7415±.0300●	.7388±.0304●	.7354±.0297●
eunite2001	.8484±.0132	.8482±.0132	.8348±.0143●	.8442±.0144●	.8349±.0150●	.8424±.0153●	.8320±.0150●
svmguide3	.2705±.0255	.2701±.0257	.2615±.0260●	.2601±.0279●	.2557±.0270●	.2136±.0325●	.2397±.0237●
ionosphere	.5995±.0326	.5990±.0329	.5920±.0352●	.5929±.0346●	.5921±.0353●	.5832±.0415●	.5740±.0348●
sonar	–	.5365±.0410	.5171±.0440●	.5138±.0432●	.5112±.0425●	.4321±.0636●	.4496±.0482●
triazines	–	.4301±.0603	.4150±.0592●	.4107±.0600●	.4073±.0591●	.3615±.0712●	.3793±.0584●
coil2000	–	.0627±.0076	.0624±.0076●	.0619±.0075●	.0619±.0075●	.0363±.0141●	.0570±.0075●
mushrooms	–	.9912±.0020	.9909±.0021●	.9909±.0022●	.9909±.0022●	.6813±.1294●	.8652±.0474●
clean1	–	.4368±.0300	.4169±.0299●	.4145±.0309●	.4132±.0315●	.1596±.0562●	.3563±.0364●
w5a	–	.3376±.0267	.3319±.0247●	.3341±.0258●	.3313±.0246●	.3342±.0276●	.2694±.0385●
gisette	–	.7265±.0098	.7001±.0116●	.6747±.0145●	.6731±.0134●	.5360±.0318●	.5709±.0123●
farm-ads	–	.4217±.0100	.4196±.0101●	.4170±.0113●	.4170±.0113●	–	.3771±.0110●
POSS: win/tie/loss	–	–	12/0/0	12/0/0	12/0/0	11/0/0	12/0/0

● denotes that POSS is significantly better by the t -test with confidence level 0.05

**Very good
in normal cases**

Summary

- Schema theorem
- No free lunch theorem
- Convergence
- Running time complexity
- How theory can help us?
- Why do theory?
- Theory vs. Experiments

Tired?



Can I do theoretical research of evolutionary algorithms?

Theoretical analysis of evolutionary algorithms is very difficult



L. Valiant

Turing Award
in 2010

Evolvability

Journal of the ACM, Vol. 56, No. 1, Article 3,
Publication date: January 2009.

Abstract. Living organisms function in accordance with complex mechanisms that operate in different ways depending on conditions. Darwin's theory of evolution suggests that such mechanisms evolved through variation guided by natural selection. However, there has existed no theory that would explain quantitatively which mechanisms can so evolve in realistic population sizes within realistic time

“there has existed no theory that would explain quantitatively which mechanisms can so evolve in realistic population sizes within realistic time ...”

- EAs: highly randomized and complex
- Problems: complicated

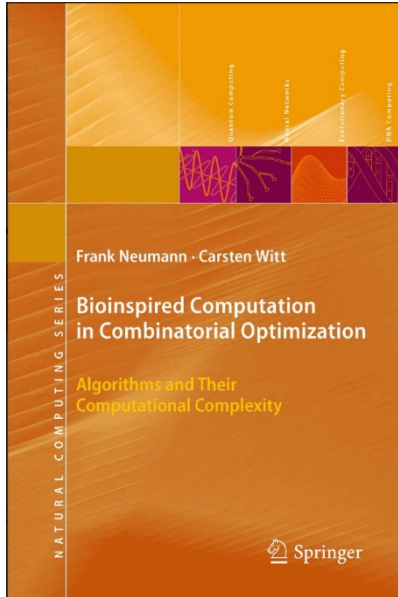
Mathematical knowledge:

- Probability Theory, Randomized Algorithms, Stochastic Processes

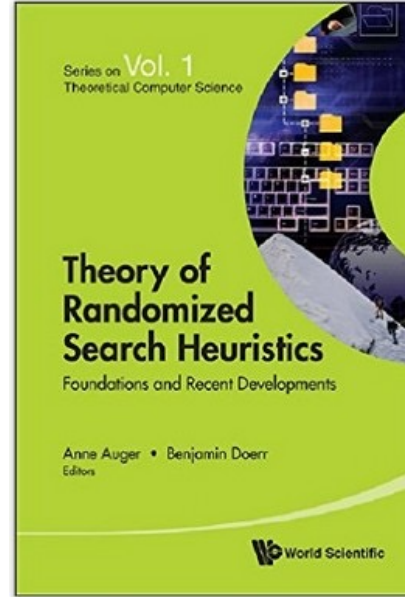
Smart: Good but not necessary!

Concentration!

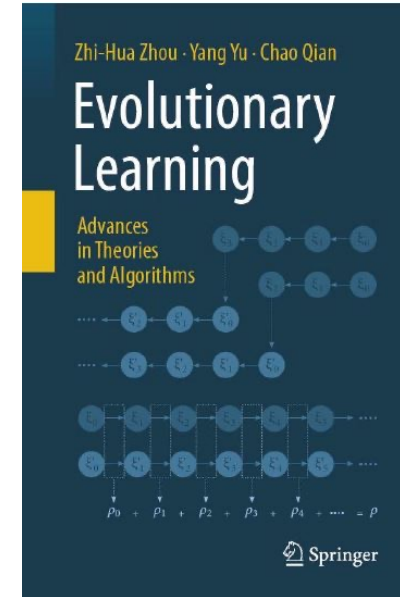
How to do theoretical research of evolutionary algorithms?



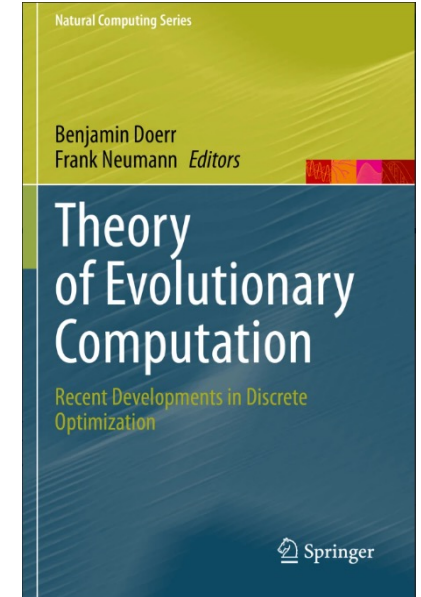
[Neumann and Witt, 2010]



[Auger and Doerr, 2011]



[Zhou, Yu and Qian, 2019]



[Doerr and Neumann, 2020]

Theoretical analysis of MOEAs may be the hottest topic in the next few years

Do useful theory!

Thank you!