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**LAMDA**  
Learning And Mining from Data  
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# Why Do We Need Theoretical Research of Evolutionary Algorithms?

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# Theory

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*“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

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## 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 01#1#
- $m(H, t)$ : number of individuals belonging to schema  $H$  in the  $t$ -th population

# Schema theorem



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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

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↓

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  $f$

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

# No free lunch theorem

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

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



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?

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### 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

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Does an EA converge to a global optimum?

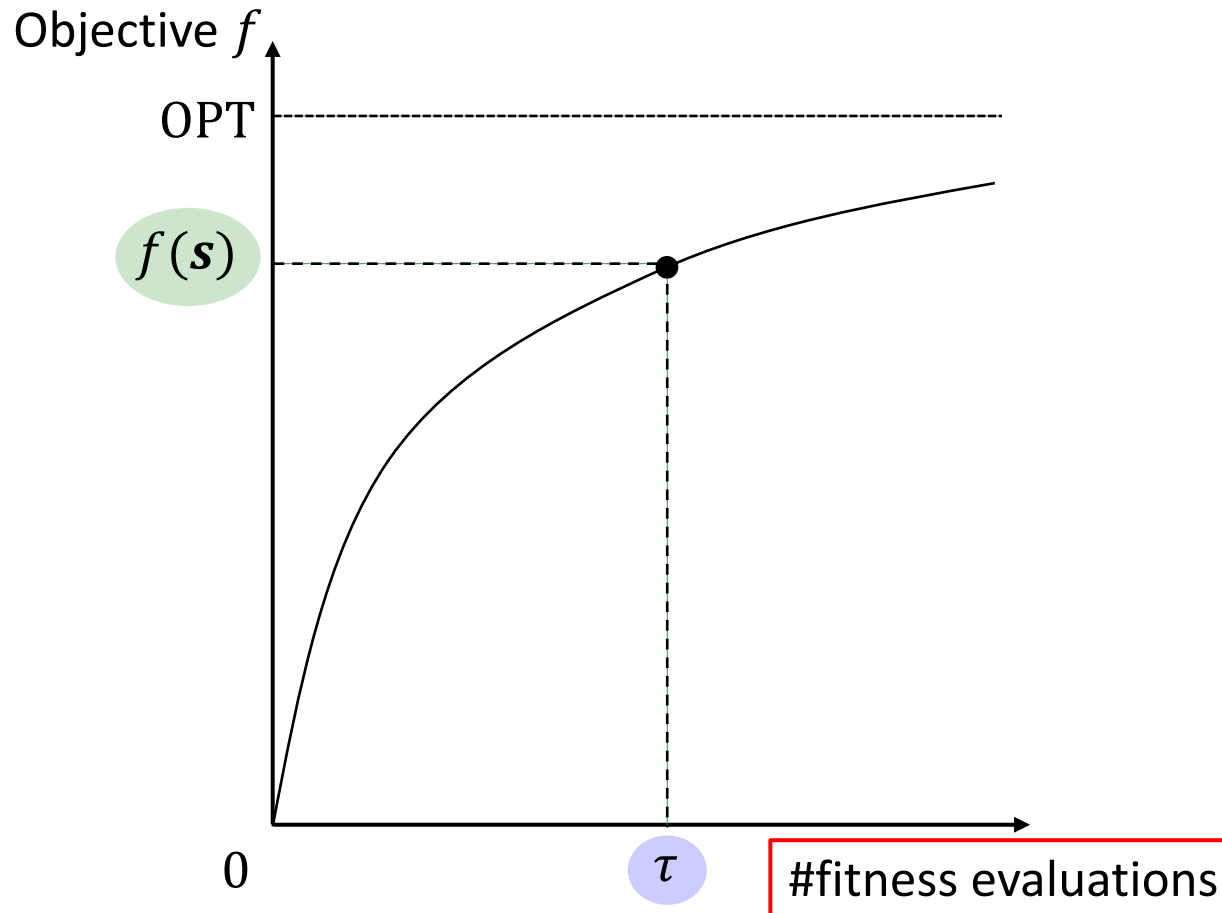
$$\lim_{t \rightarrow +\infty} P(\xi_t \in \mathcal{X}^*) = 1$$

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



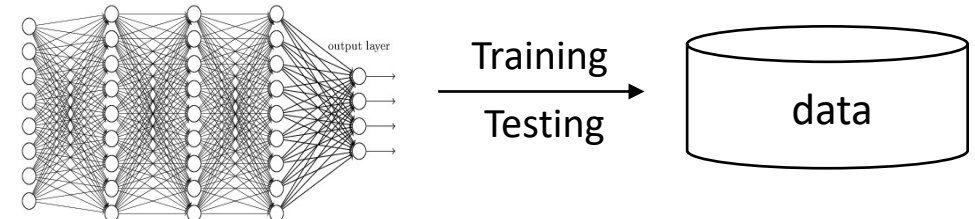
What we concern:

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

Running time  $\tau$ :

#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

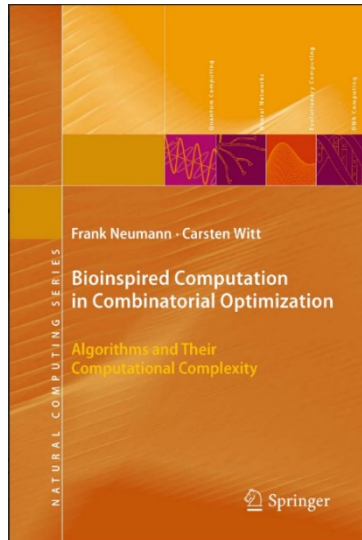
Drift Analysis  
[He & Yao, AIJ'01]



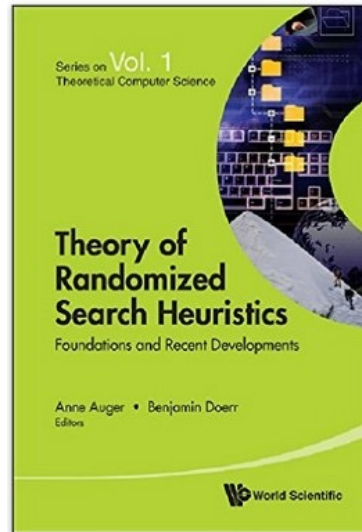
**X. Yao**  
SUSTech, China  
IEEE Frank Rosenblatt Award

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

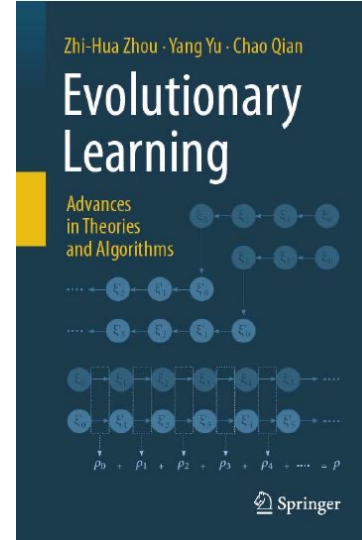
*Stefan Droste, Thomas Jansen, Ingo Wegener:  
A Rigorous Complexity Analysis of the (1 + 1) Evolutionary Algorithm for Separable Functions with Boolean Inputs.  
Evolutionary Computation 6(2): 185-196 (1998)*



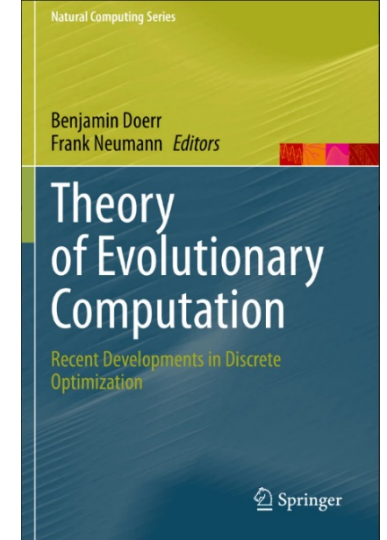
[Neumann and Witt, 2010]



[Auger and Doerr, 2011]



[Zhou, Yu and Qian, 2019]



[Doerr and Neumann, 2020]

## How running time analysis can help us?

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

## Example illustration: Help understand behaviors of EAs

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**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**

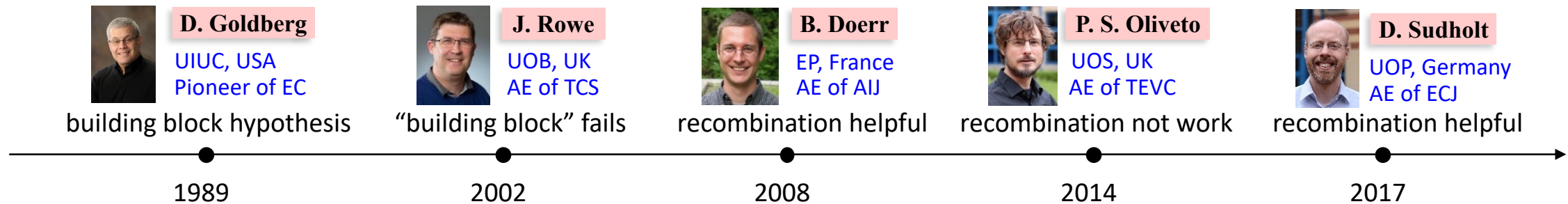
**More complicated**



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

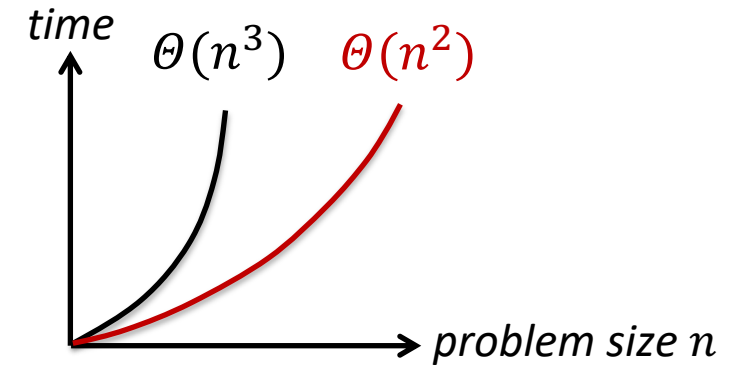
How about the influence of recombination for **multi-objective optimization?**

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

## Example illustration: Help understand behaviors of EAs

**Theorem:** For GSEMO solving the LOTZ problem

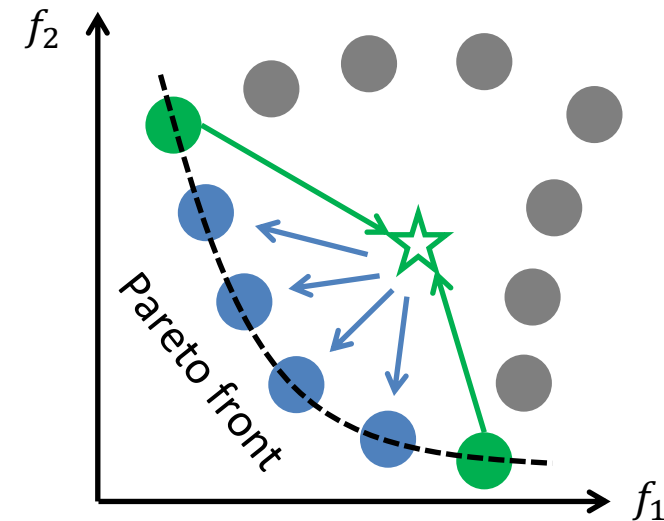
Expected running time  $\Theta(n^3)$   $\xrightarrow{\text{recombination}}$   $\Theta(n^2)$



### 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

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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, ....

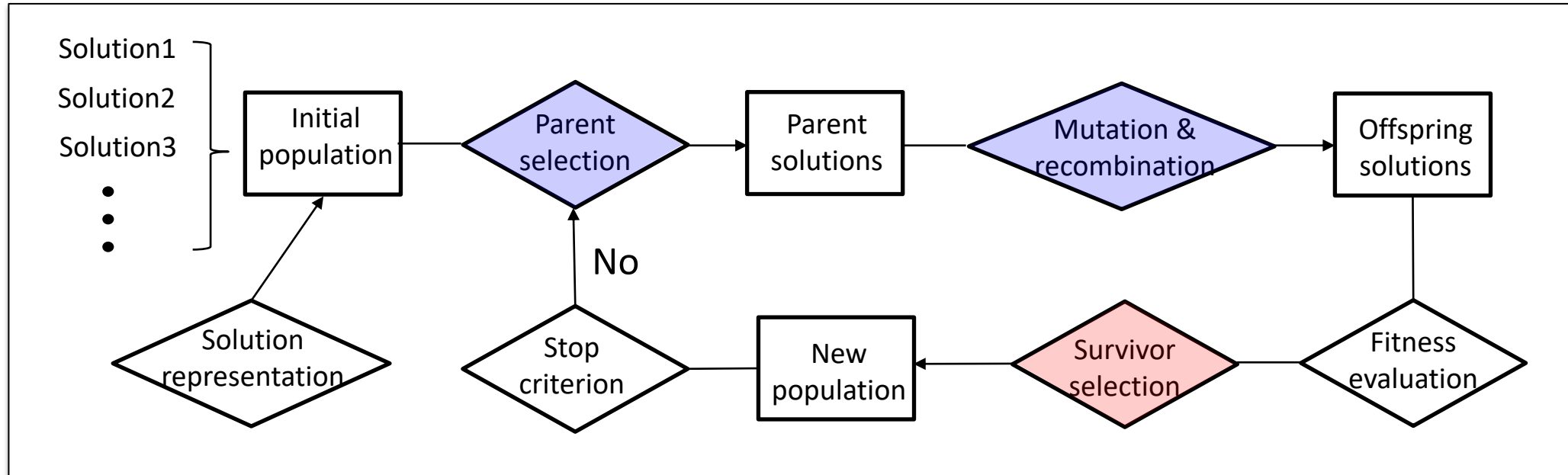


Q. Zhang and H. Li. MOEA/D: A multiobjective evolutionary algorithm based on decomposition. *IEEE Transactions on Evolutionary Computation*, 2007. (Google scholar citations: 7515)



## Example illustration: Guide the design of EAs

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

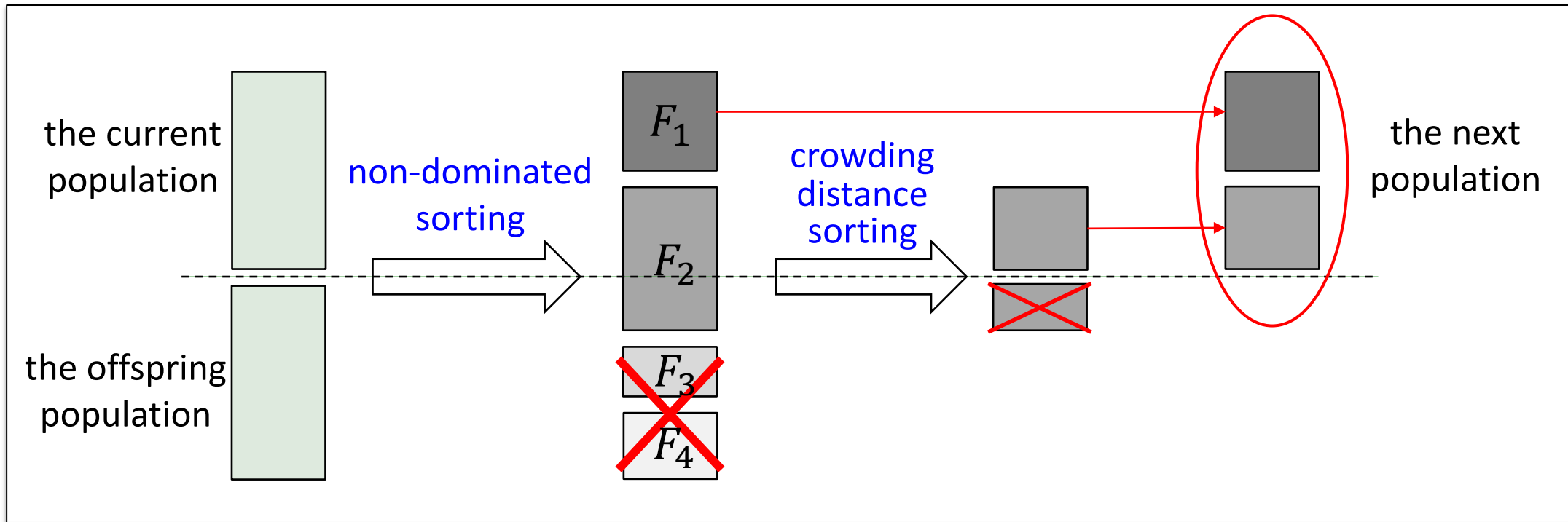


In the area of evolutionary multi-objective optimization, the research focus is mainly on population update

## Example illustration: Guide the design of EAs

### Population Update of NSGA-II:

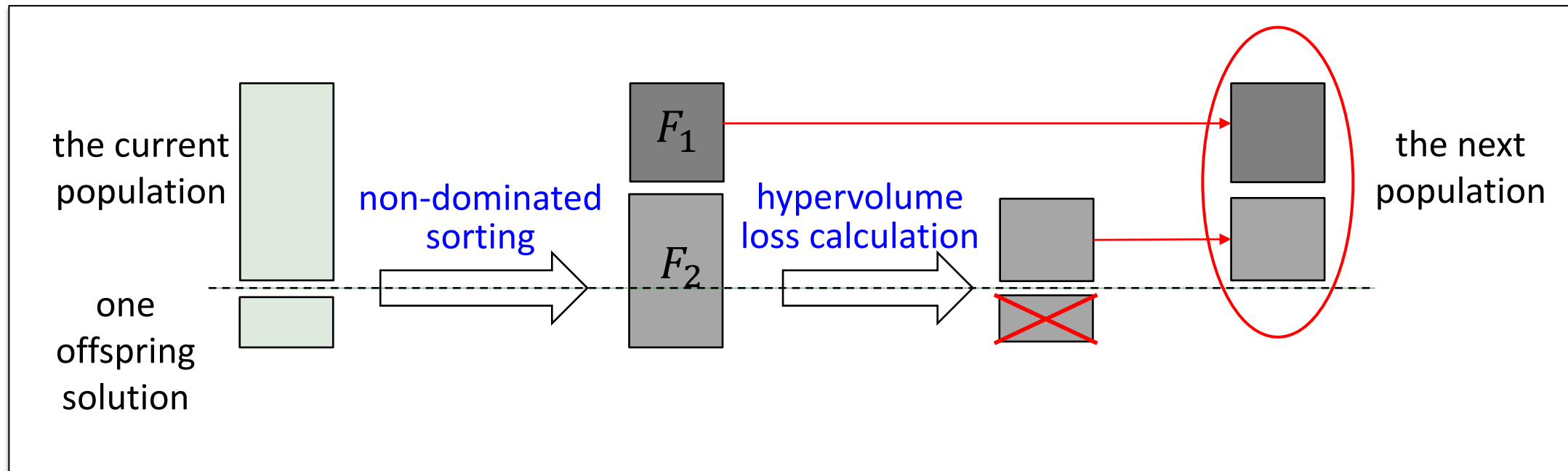
Use **non-dominated sorting** and **crowding distance sorting** to rank the solutions, and **delete the worst ones**



## Example illustration: Guide the design of EAs

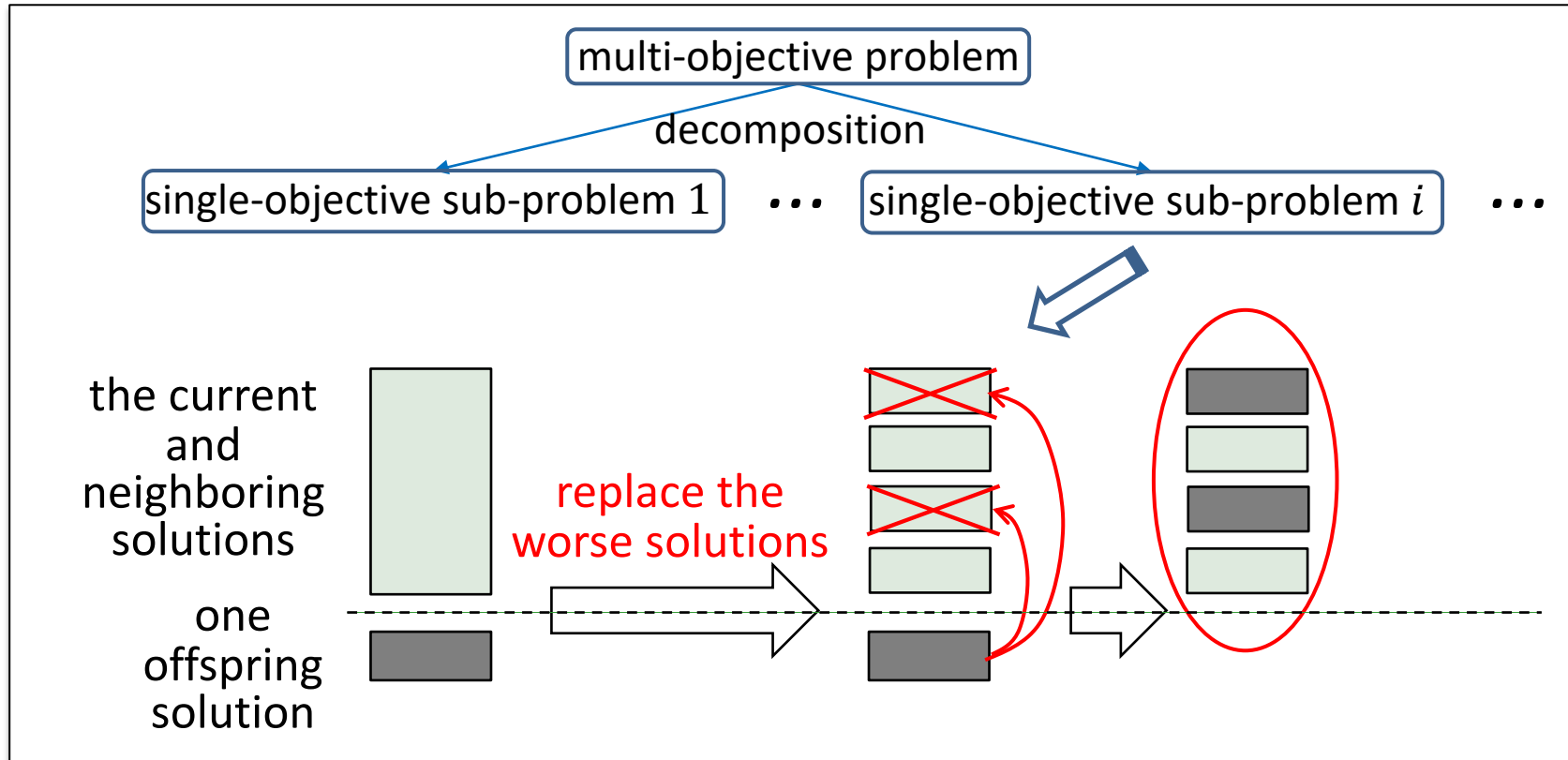
### Population Update of SMS-EMOA:

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

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The prominent feature in population update of MOEAs: **Elitism**

- 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*

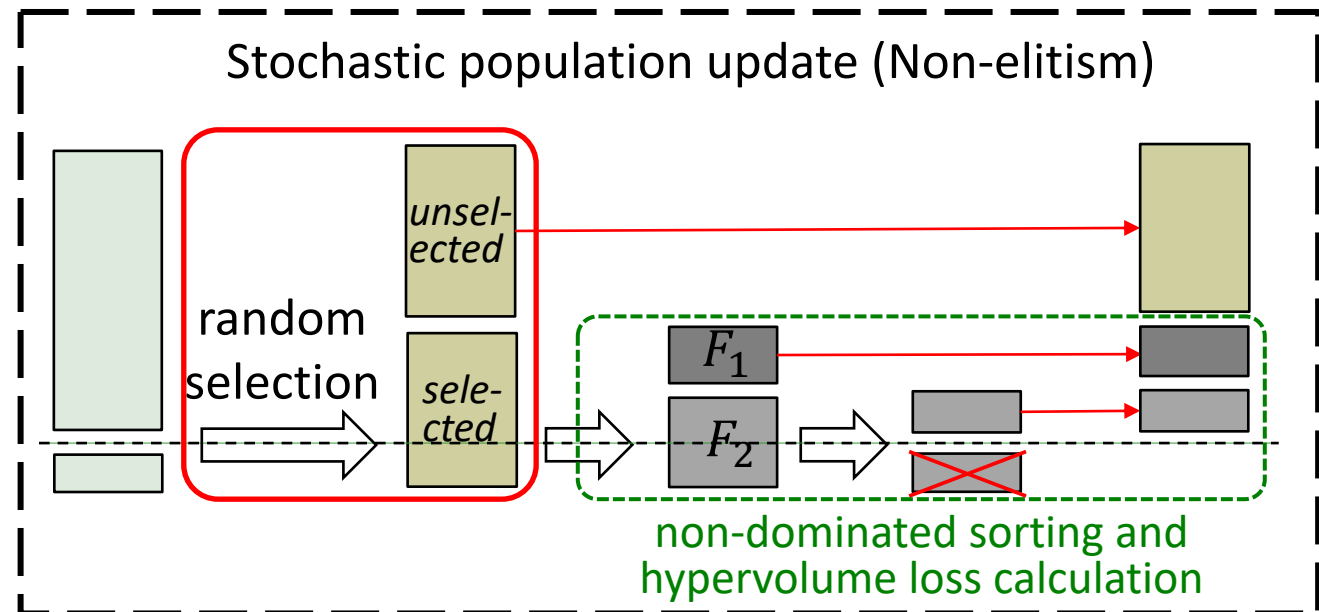
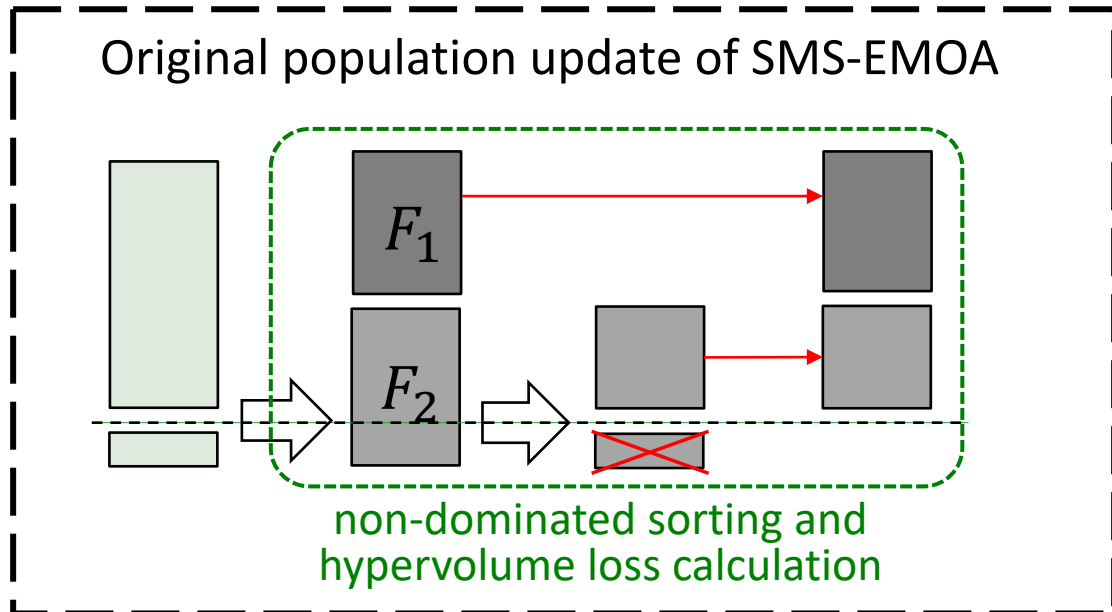
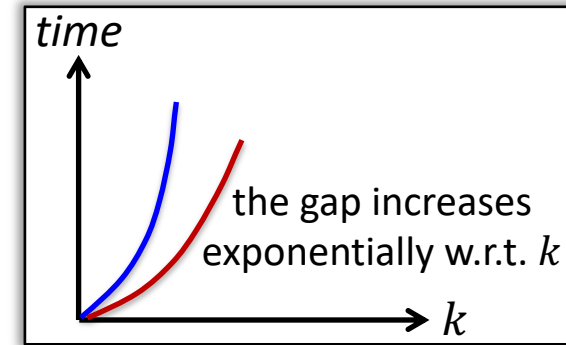
Is elitist population update always better?

**NO!**

# Example illustration: Guide the design of EAs

**Theorem:** For SMS-EMOA solving the OneJumpZeroJump problem

Expected running time  $\Omega(n^k)$  Non-elitism  
accelerate by  $2^{k/4}/\mu^2$   $\rightarrow$   $O(\mu n^k \cdot \min\{1, \mu/2^{k/4}\})$   
exponentially faster



## 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

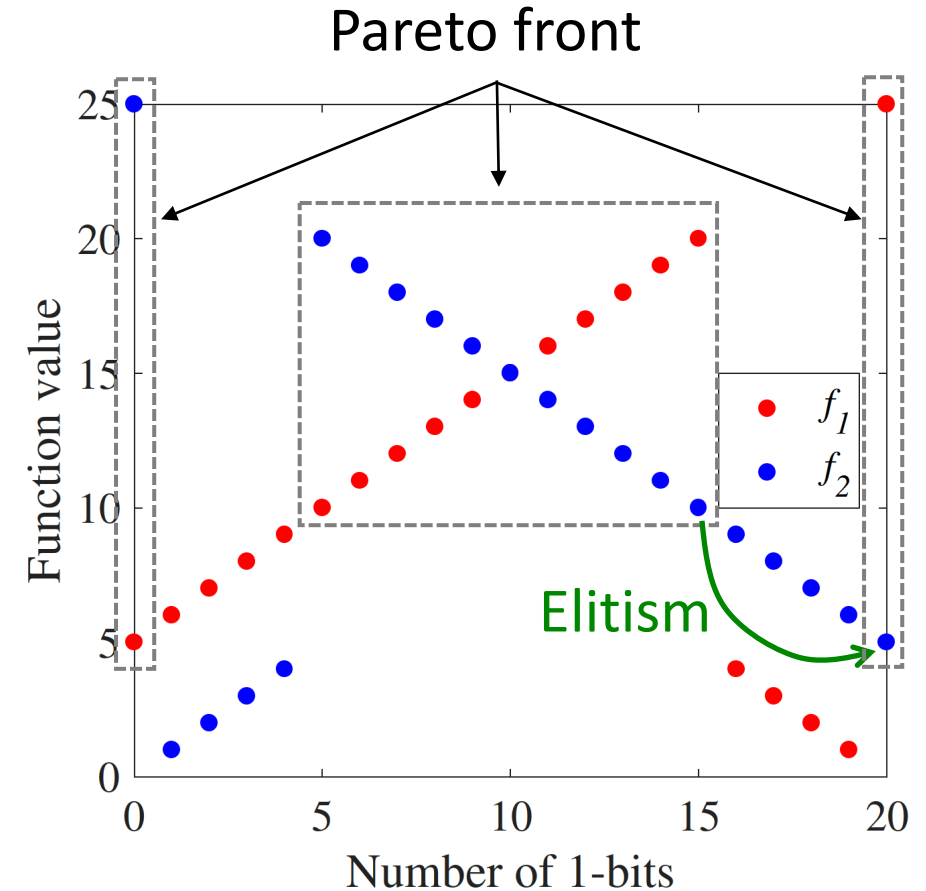


Illustration of function values  
when  $n = 20$  and  $k = 5$

## Example illustration: Guide the design of EAs

The OneJumpZeroJump problem:

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

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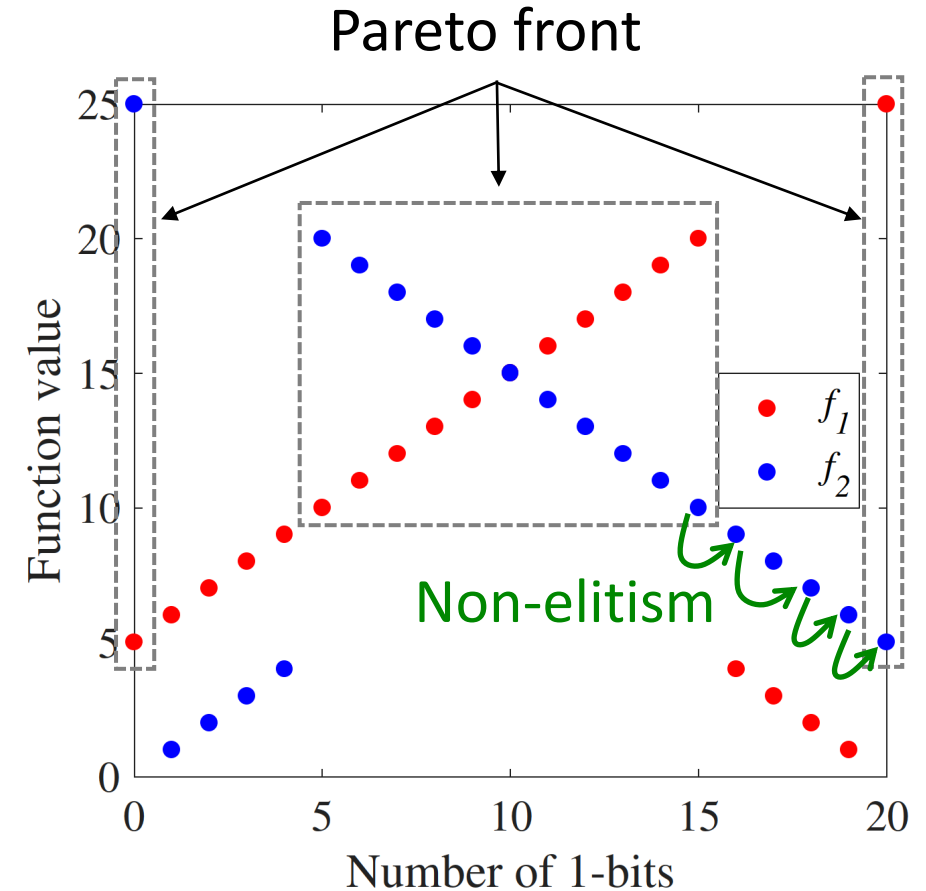


Illustration of function values  
when  $n = 20$  and  $k = 5$



## Example illustration: Guide the design of EAs

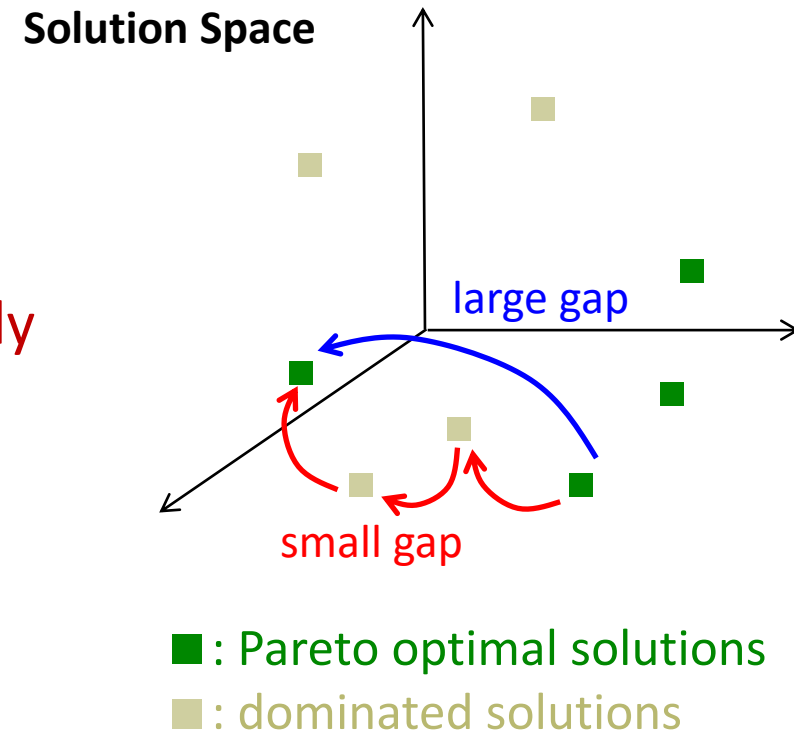
Non-elitism can make MOEAs go across inferior regions between different Pareto optimal solutions more easily, thus facilitating to find the whole Pareto front

### ➤ Elitism

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

### ➤ Non-elitism May hold more generally

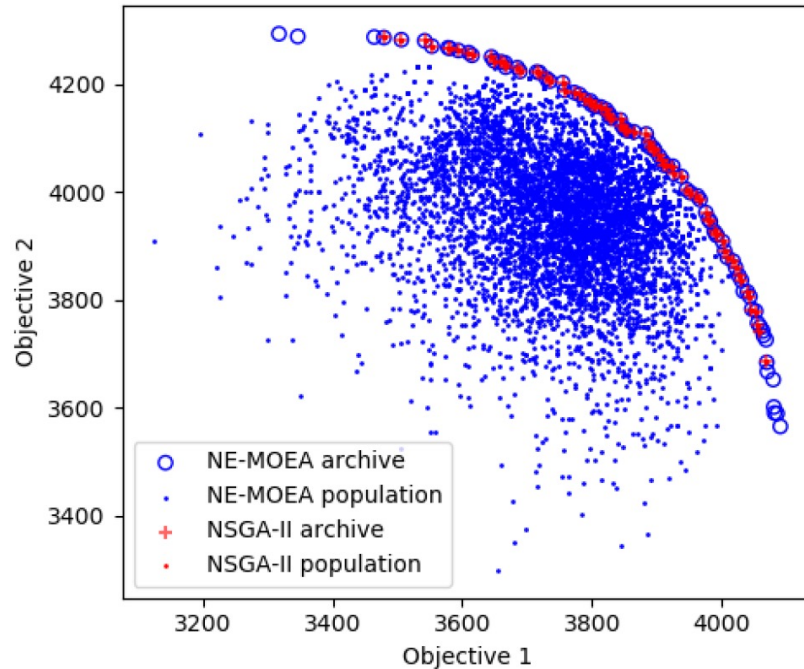
- allows dominated solutions to participate in the evolutionary process
- may follow an easier path in the solution space to find points in the Pareto front



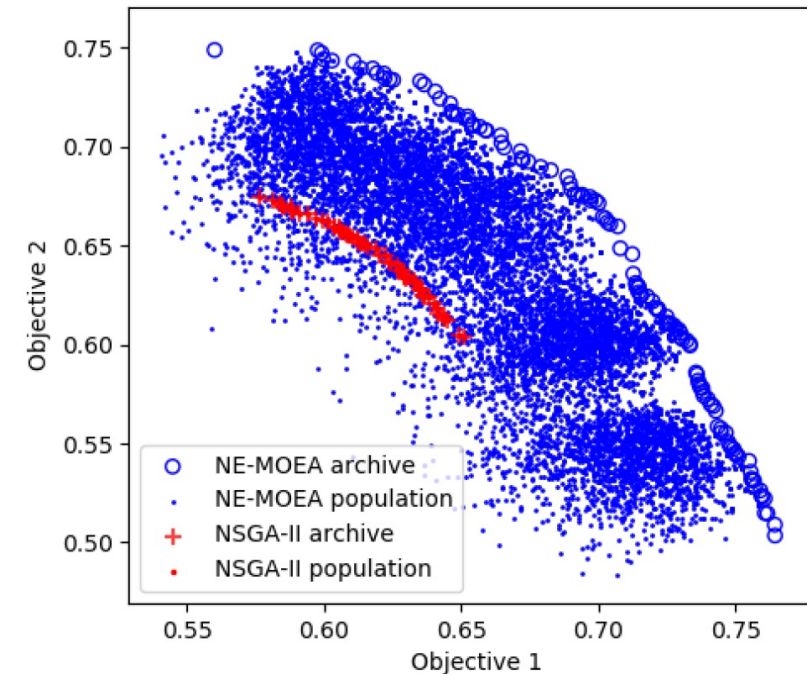
## Example illustration: Guide the design of EAs

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

observation variables      predictor variable

	Corr.	Dis.	LR	...	...	AIC.	BIC	RF.
x1	0.28	0.46	1	...	...	0.22	0.63	1
x2	0.31	0.59	0.64	...	...	0.58	0.56	1
x3	0.11	0.02	0.53	...	...	0.43	0.01	1
x4	0.1	0.1	0.64	...	...	0.73	0.92	1
x5	0.02	0.15	0.33	...	...	0.56	0.36	0.78
x6	0.36	0.02	0.01	...	...	0.32	0.02	0.22
x7	0.2	0.2	0.21	...	...	0.21	0.02	0.11
x8	0.1	0.03	0.32	...	...	0.33	0.51	0.44
x9	0.32	0.1	0.2	...	...	0.06	0.66	0
x10	0.24	0	0.02	...	...	0.6	0.03	0.33
x11	0.12	0.45	0.44	...	...	0.64	0.45	1
x12	0.36	0.58	0.12	...	...	0.73	0.58	0.67
x13	0.2	0.02	0.24	...	...	0.34	0.02	0.89
x14	0.24	0.92	0.33	...	...	0.24	0.93	0.56

Feature selection



a subset of observation variables

	Corr.	Dis.	LR	...	...	AIC.	BIC	RF.
x1	0.28	0.46	1	...	...	0.22	0.63	1
x2	0.31	0.59	0.64	...	...	0.58	0.56	1
x3	0.11	0.02	0.53	...	...	0.43	0.01	1
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x5	0.02	0.15	0.33	...	...	0.56	0.36	0.78
x6	0.36	0.02	0.01	...	...	0.32	0.02	0.22
x7	0.2	0.2	0.21	...	...	0.21	0.02	0.11
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x10	0.24	0	0.02	...	...	0.6	0.03	0.33
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# Example illustration: Generate EAs with theoretical guarantees

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

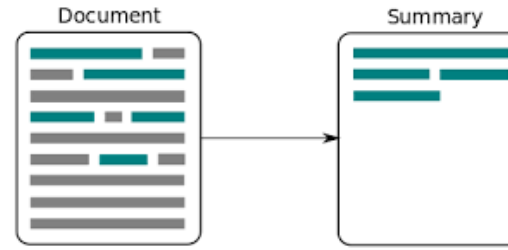
Sparse regression

	Corr	Dis	L1	...	...	AIC	BIC	R <sup>2</sup>
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	0.4	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	0.6	0.22
x7	0.2	0.2	0.21	...	...	0.21	0.6	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	0.6	0.33
x11	0.12	0.45	0.44	...	...	0.64	0.4	1
x12	0.36	0.58	0.12	...	...	0.73	0.5	0.67
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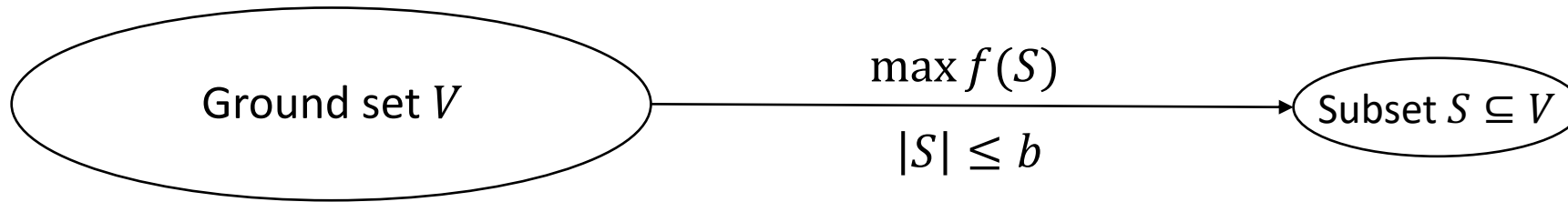
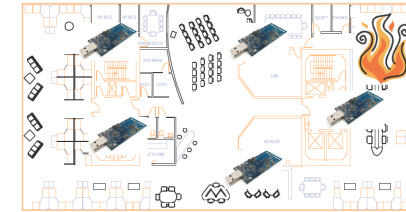
Influence maximization



Document summarization



Sensor placement



**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)

Constrained Transformation Bi-objective

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

**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  $\mathbf{s} \in \{0, 1\}^n$  with  $|\mathbf{s}|_1 \leq b$

**Process:**

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

**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  $\gamma_{\min} = \min_{s:|s|_1=b-1} \gamma_{s,b}$ .

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

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

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	?

Experiments

Guaranteed

Safe!

Remark: Theoretical guarantee implies worst-case performance

## Example illustration: Generate EAs with theoretical guarantees

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[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  $\beta$ -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

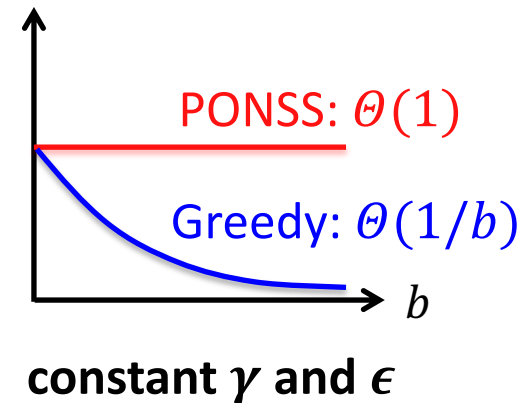


**Greedy** [Horel and Singer, NIPS'16]



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

approximation ratio



EAs achieve better approximation guarantees than conventional algorithms



## How running time analysis can help us?

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

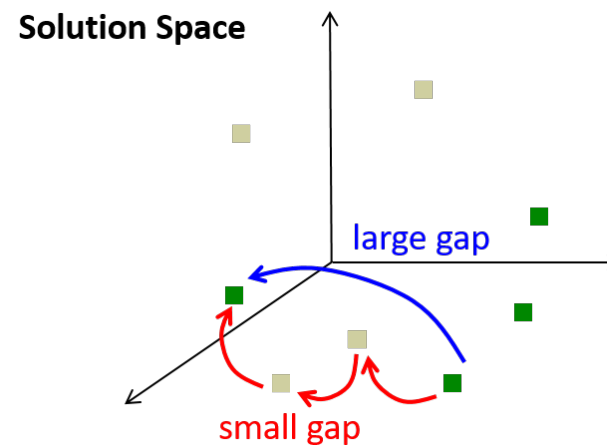
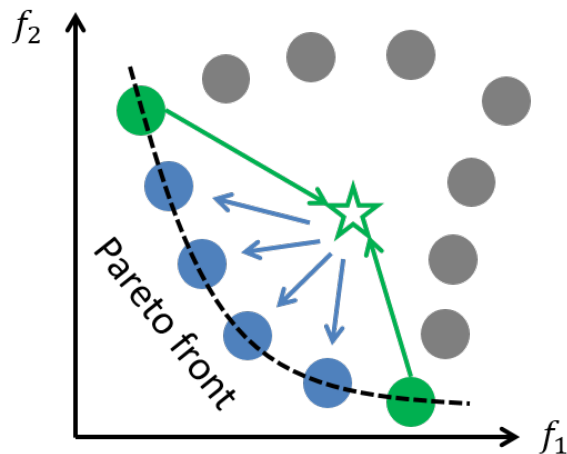
# Why do theory?

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

---

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**Not bad in the worst case**

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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●
svmguid3	.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

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- 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?

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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

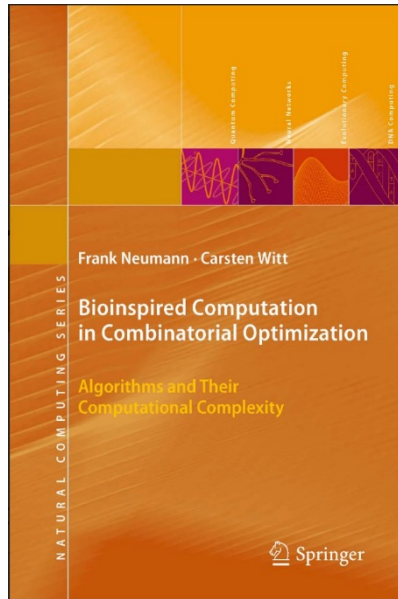
Smart: Good but not necessary!

**Concentration!**

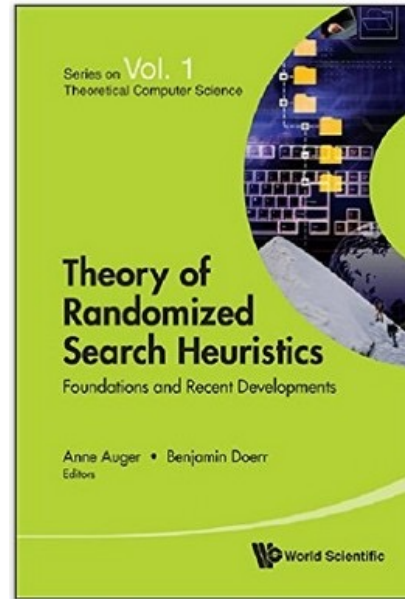


# How to do theoretical research of evolutionary algorithms?

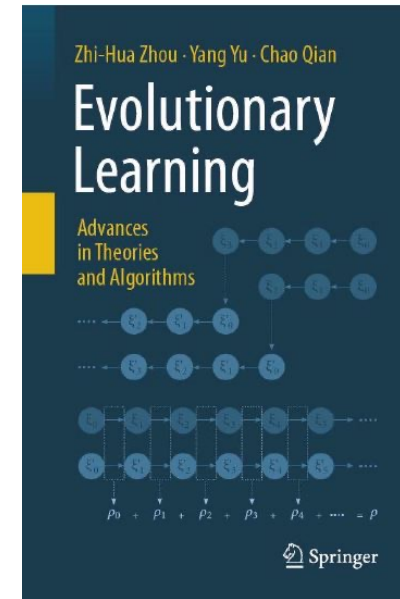
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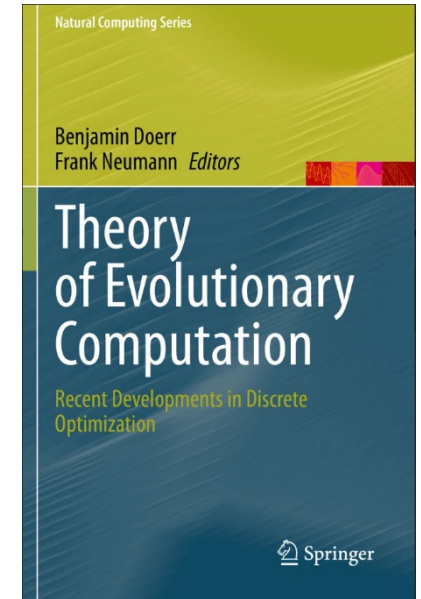
[Neumann and Witt, 2010]



[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!**