8-12 July 2020

Surrogate-assisted Multi-objective Combinatorial Optimization based on Decomposition and Walsh Basis

Geoffrey Pruvost, Bilel Derbel, Arnaud Liefooghe, Sébastien Verel, Qingfu Zhang

Université de Lille

CRIStAL
Centre de Recherche en Informatique, Signal et Automatique de Lille

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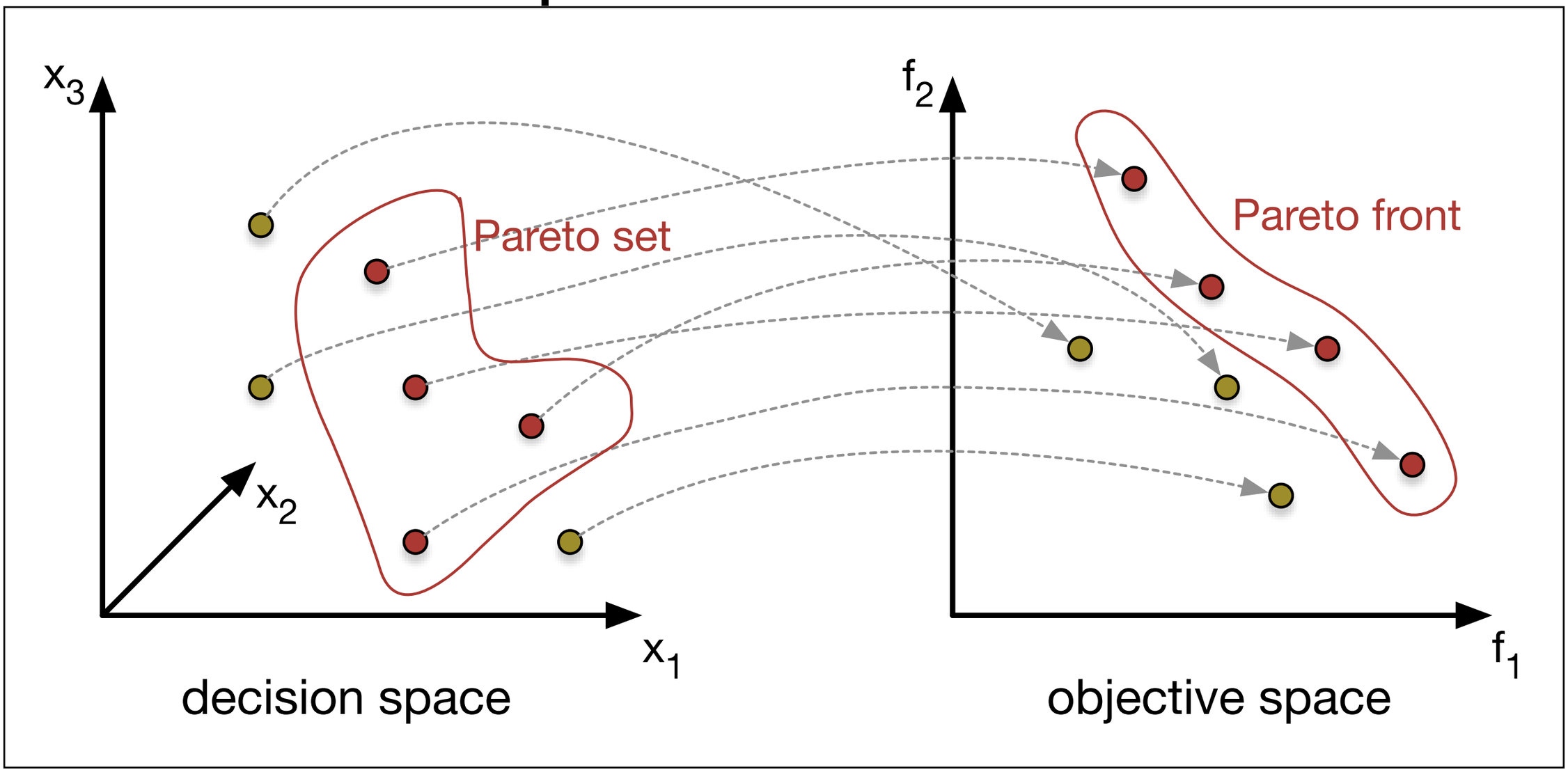
Outline

- General Context
  - Multi-Objective Optimization
  - Surrogates for combinatorial problems
- Design and analysis of the new *S-CMO Framework* for *pseudo-boolean functions*
- Experimental study and main results
- Conclusion

Multi-objective optimization



- Conflicting objectives
- **Pareto set/front**

Find a good **Pareto set/front** approximation

Expensive Optimization

$$x \xrightarrow{\text{expensive function}} F(x)$$

Example :

- heavy simulation in industry
- road traffic simulation

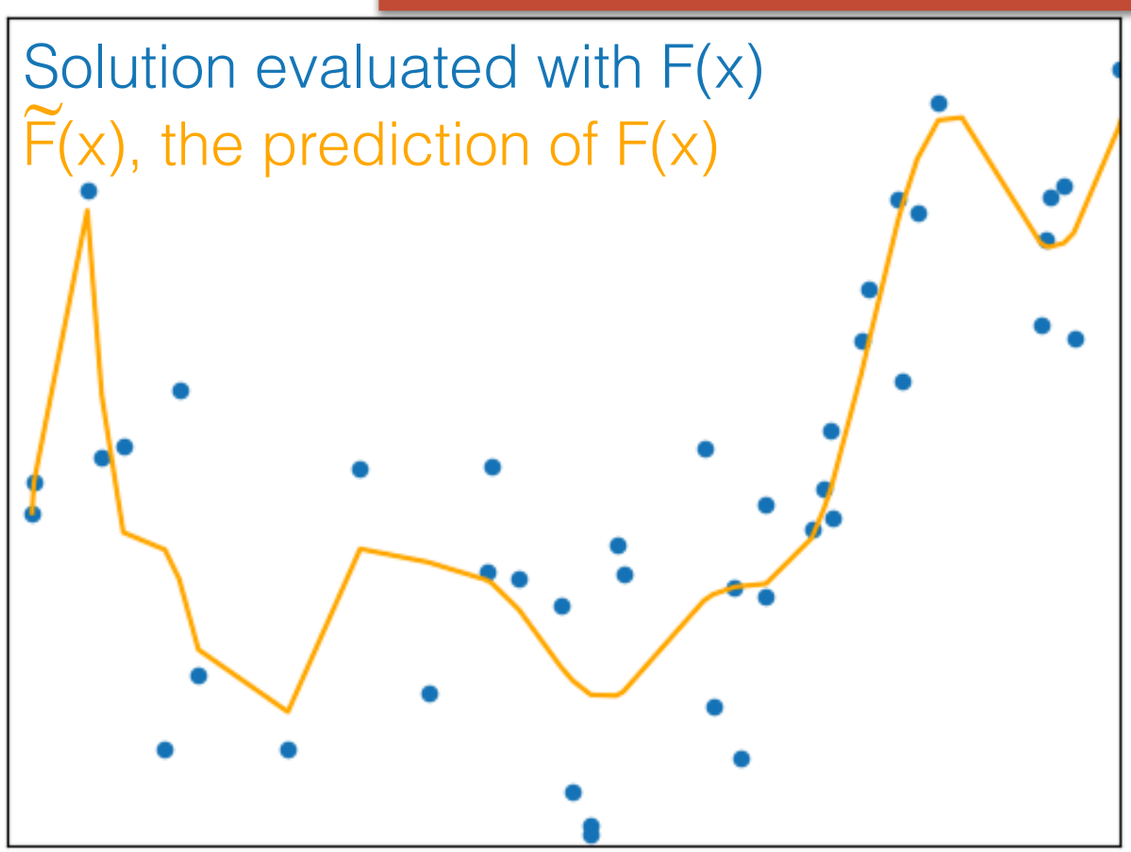
Consequence :

- A low number of evaluation

Expensive Optimization

$$x \xrightarrow{\text{expensive function}} F(x)$$

$$x \xrightarrow{\text{Surrogate model}} \tilde{F}(x)$$



Surrogate model :

- Cheap alternative
- Prediction of F(x)

Advantage	Disadvantage
Faster	Reduced quality

Expensive Optimization Discrete Surrogates

- Extensions of numerical models :
  - ➡ RBF
  - ➡ Kriging
  - ➡ Bocs

- A new model :
  - ➡ Walsh[1]

    Competitive[2] compared against BOCS, Krigging and RBF

[1] Sébastien Verel et al. A surrogate model based on Walsh decomposition for pseudo-boolean functions. PPSN 2018

[2] Florian Leprêtre et al. Walsh functions as surrogate model for pseudo-boolean optimization problems. GECCO 2019

Walsh Surrogates

- Walsh functions : set of functions $\phi_k : [0,1] \rightarrow \{-1,1\}$
- Decompose any function of the Hilbert space
- f can be approximated by the following model :

$$\forall x \in \{0,1\}^n,\ \tilde{f}(x|d) = \sum_{k\,:\,o(\phi_k)\leqslant d} \widetilde{w}_k.\phi_k(x)$$

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Walsh function

Coefficient

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Walsh function

Coefficient

Walsh order

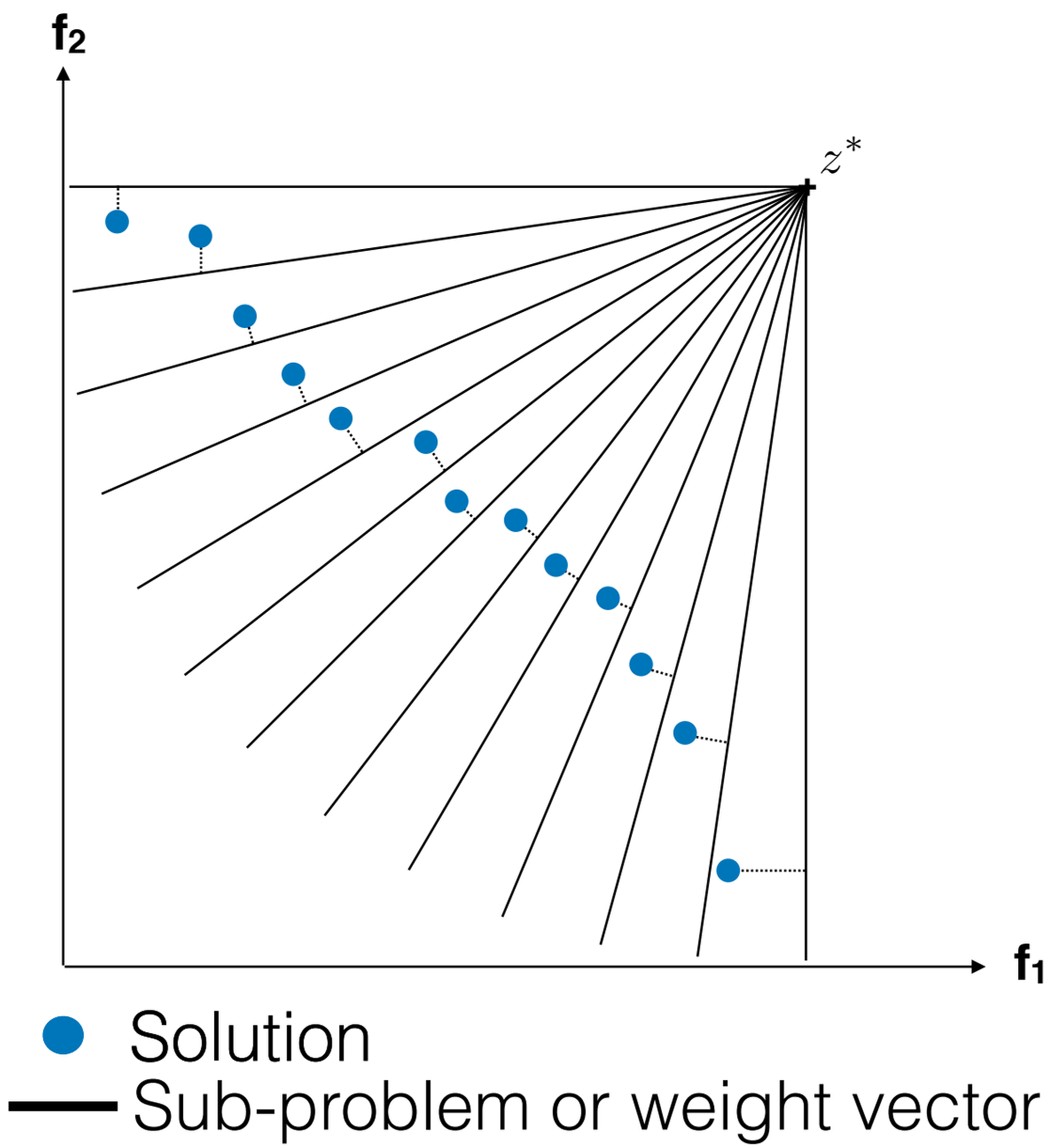
The S-CMO Framework
Based on MOEA/D

Surrogate-assisted Combinatorial Multi-objective Optimization Framework

- **Decomposition**
  - Weight vectors
  - Aggregation function

    Chebychev :

$$g(x, \lambda | z^*) \quad \max_{i \in \{1,\ldots,m\}} \lambda_i \cdot |f_i(x) - z_i^*|$$



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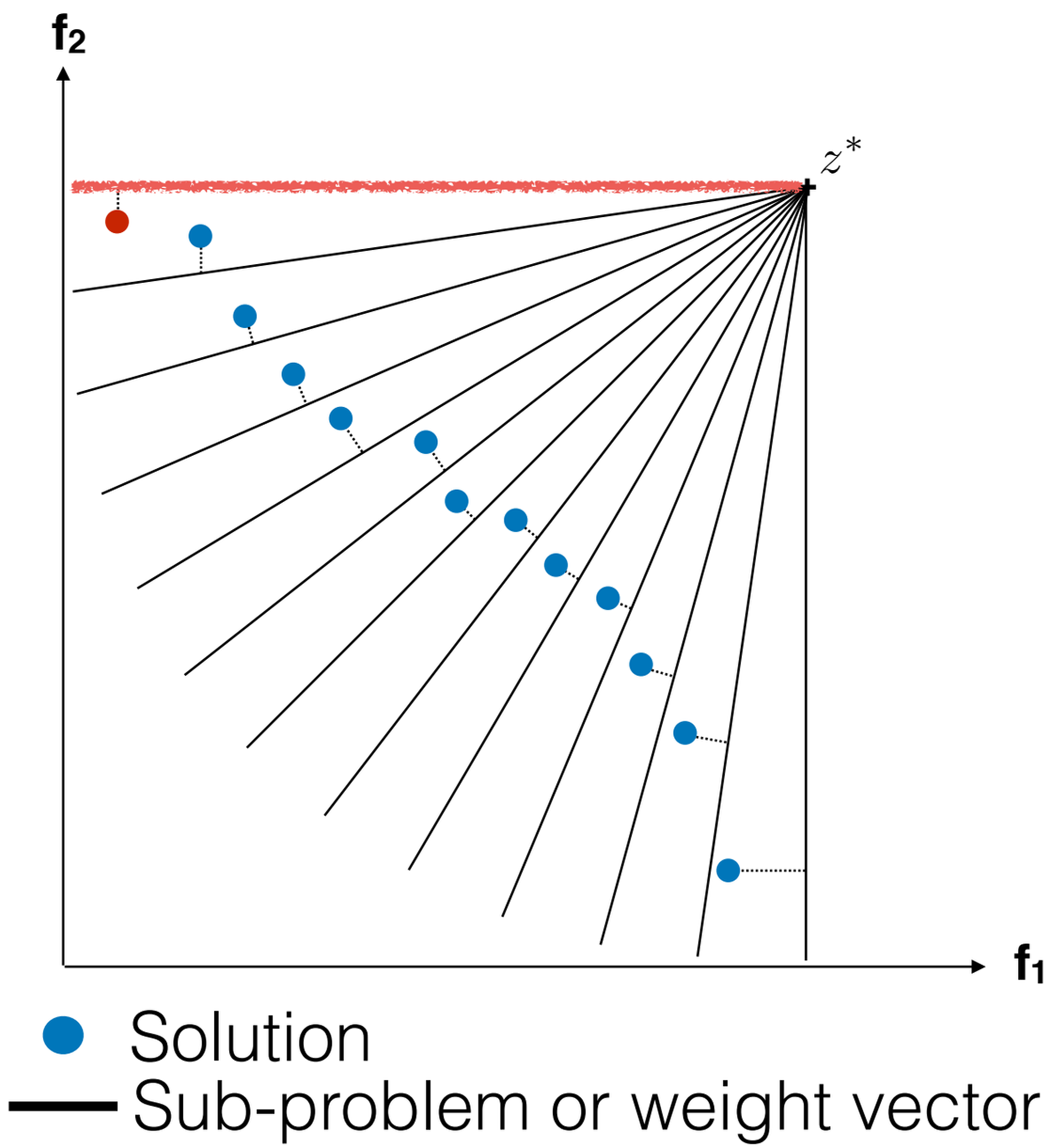

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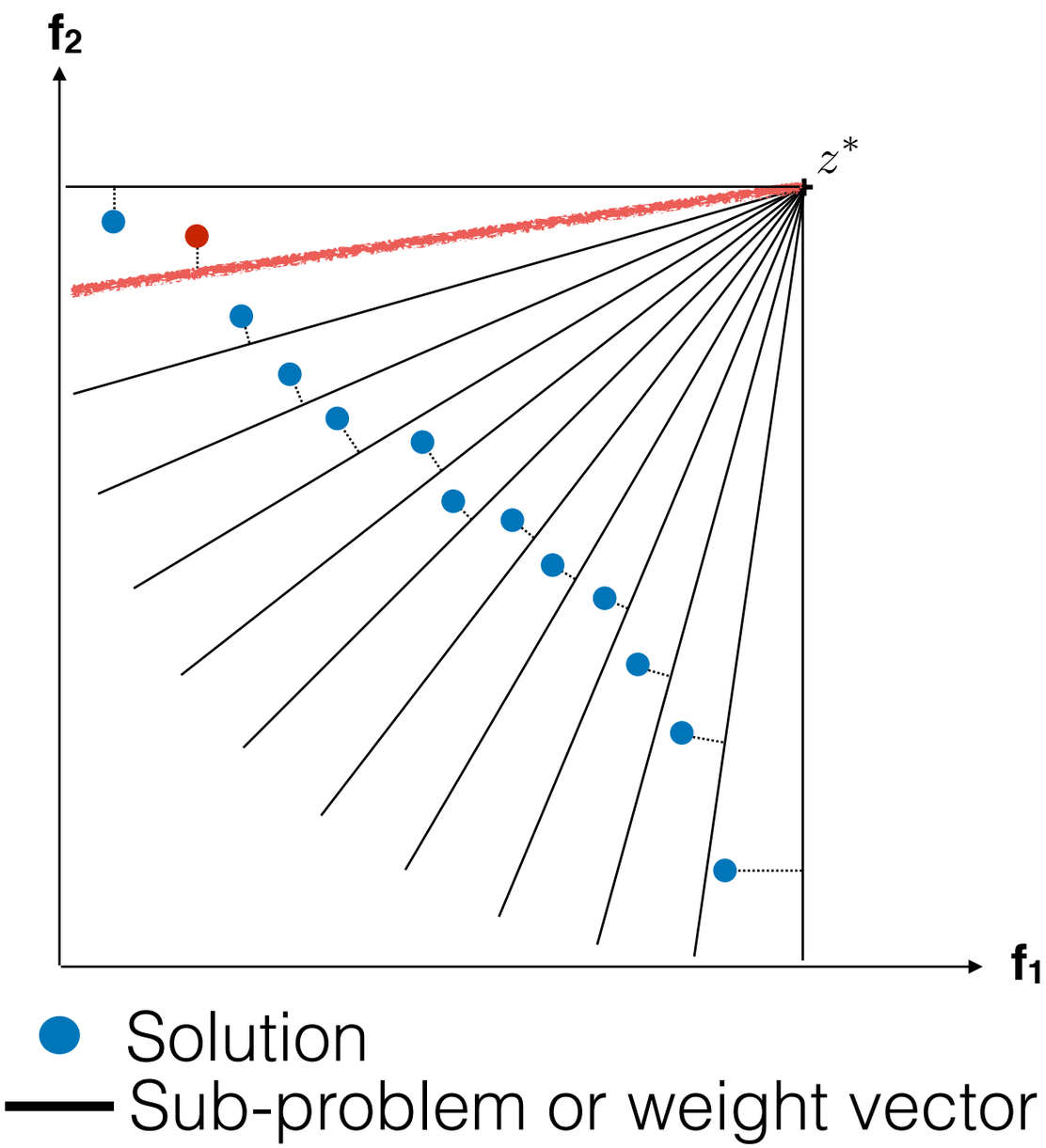

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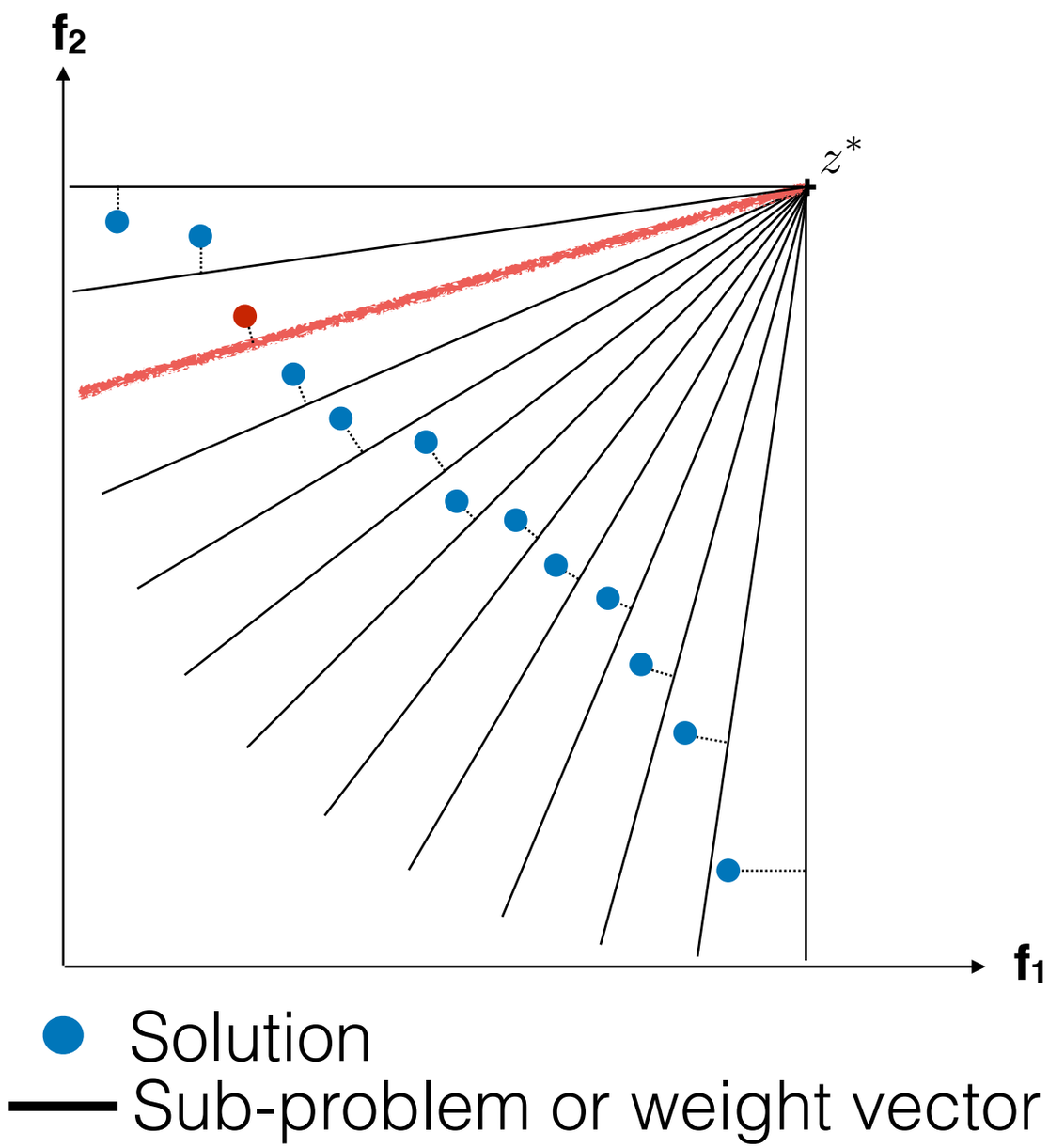

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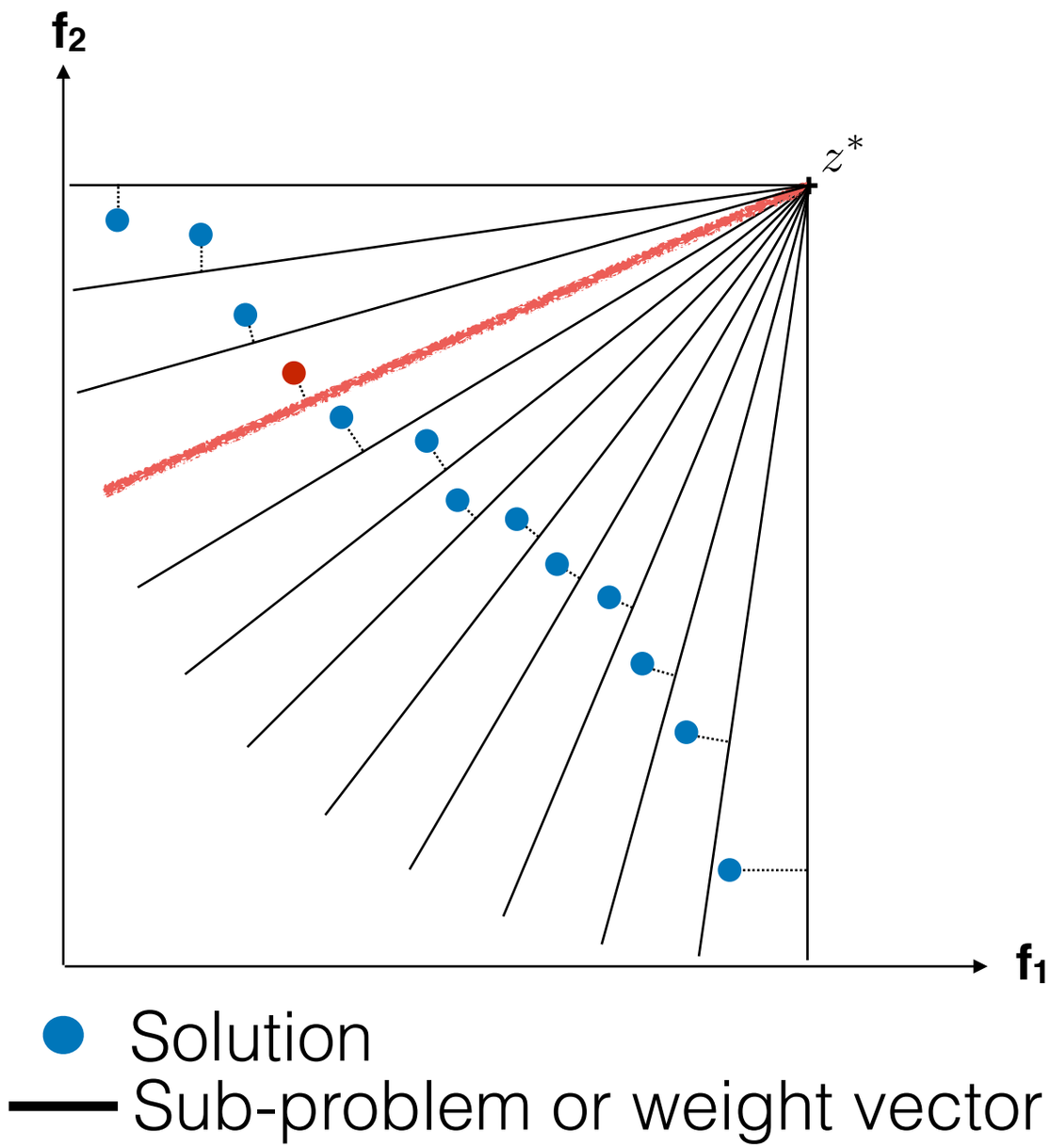

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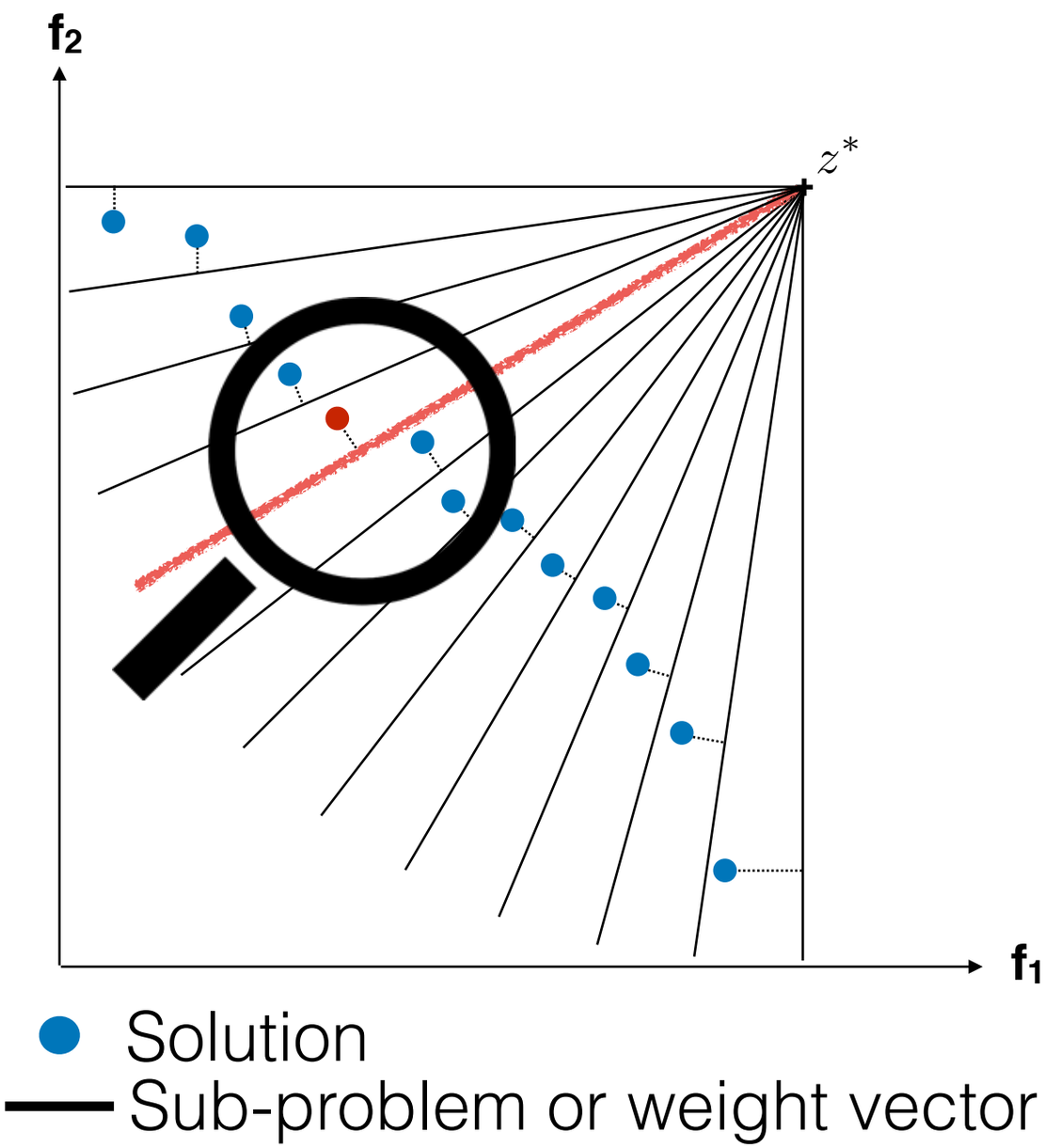
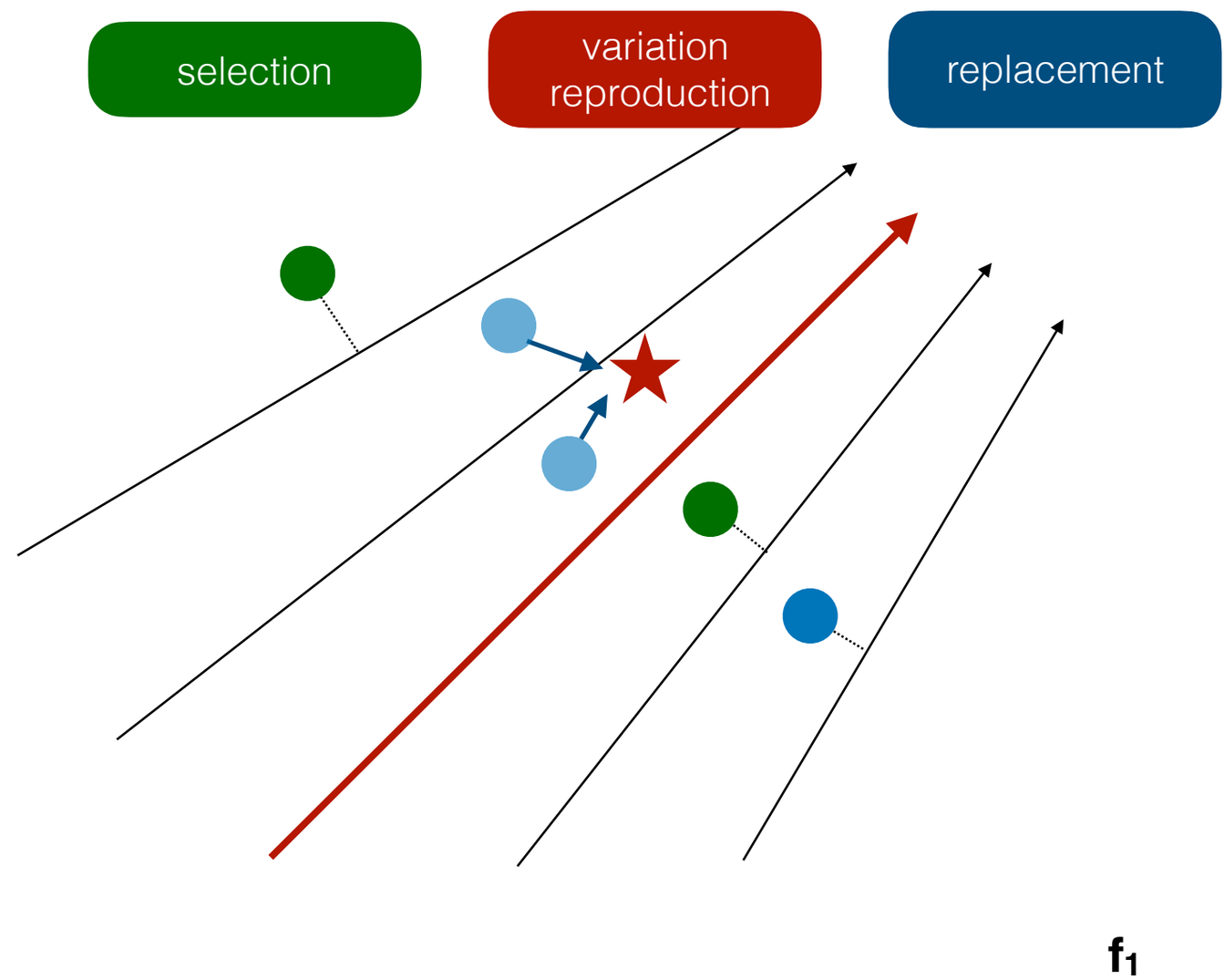


The S-CMO Framework
Based on MOEA/D

Surrogate-assisted Combinatorial Multi-objective Optimization Framework

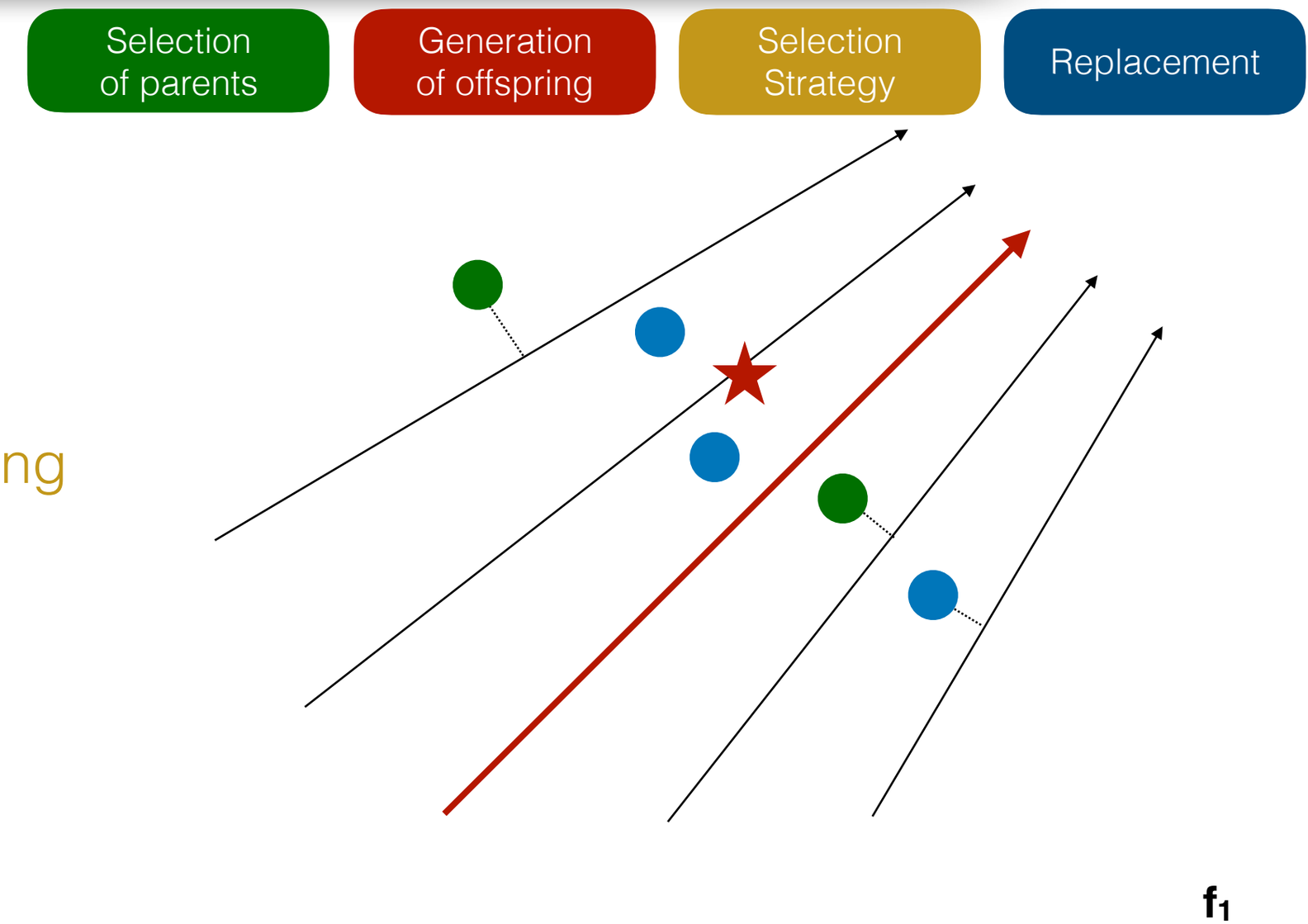
- The process in **MOEA/D**
  - Selection of Parents
  - Generate a new solution
  - Replacement by using the aggregation function



The S-CMO Framework

Surrogate-assisted Combinatorial Multi-objective Optimization Framework

- **Idea to improve the convergence**
  - Generate more than 1 offspring
  - Choose the best offspring **<u>without evaluation</u> !**
  - Classic replacement



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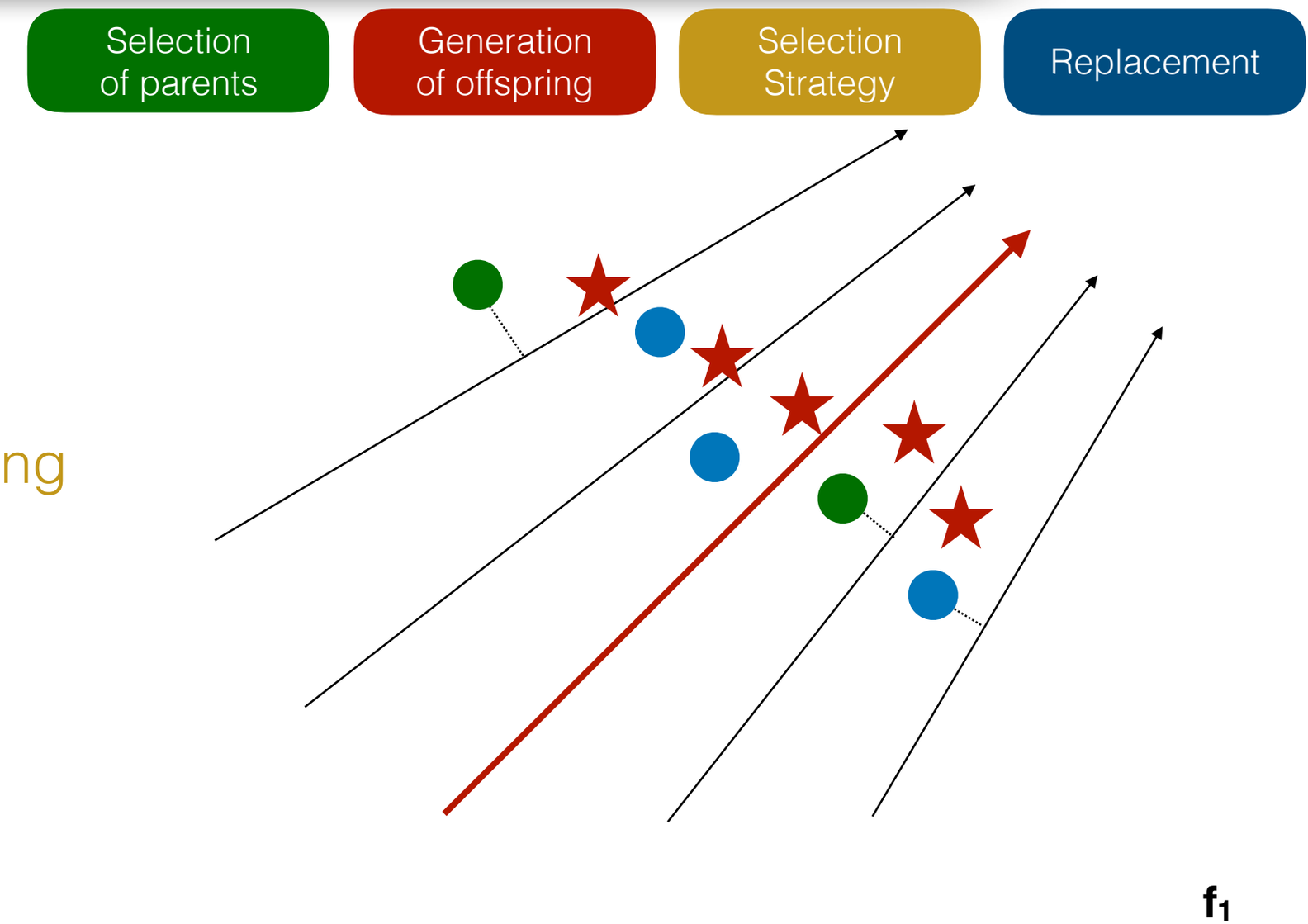

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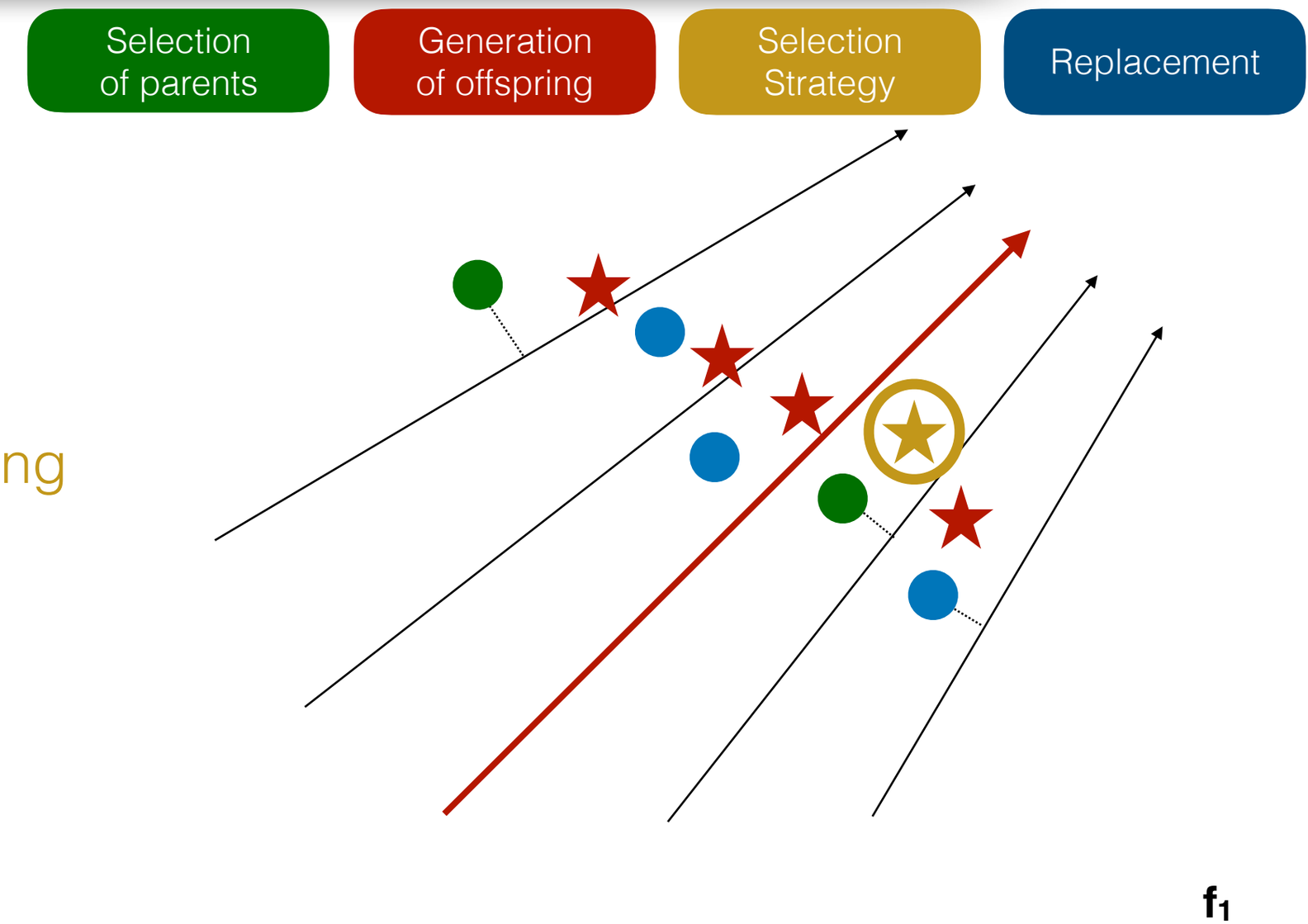

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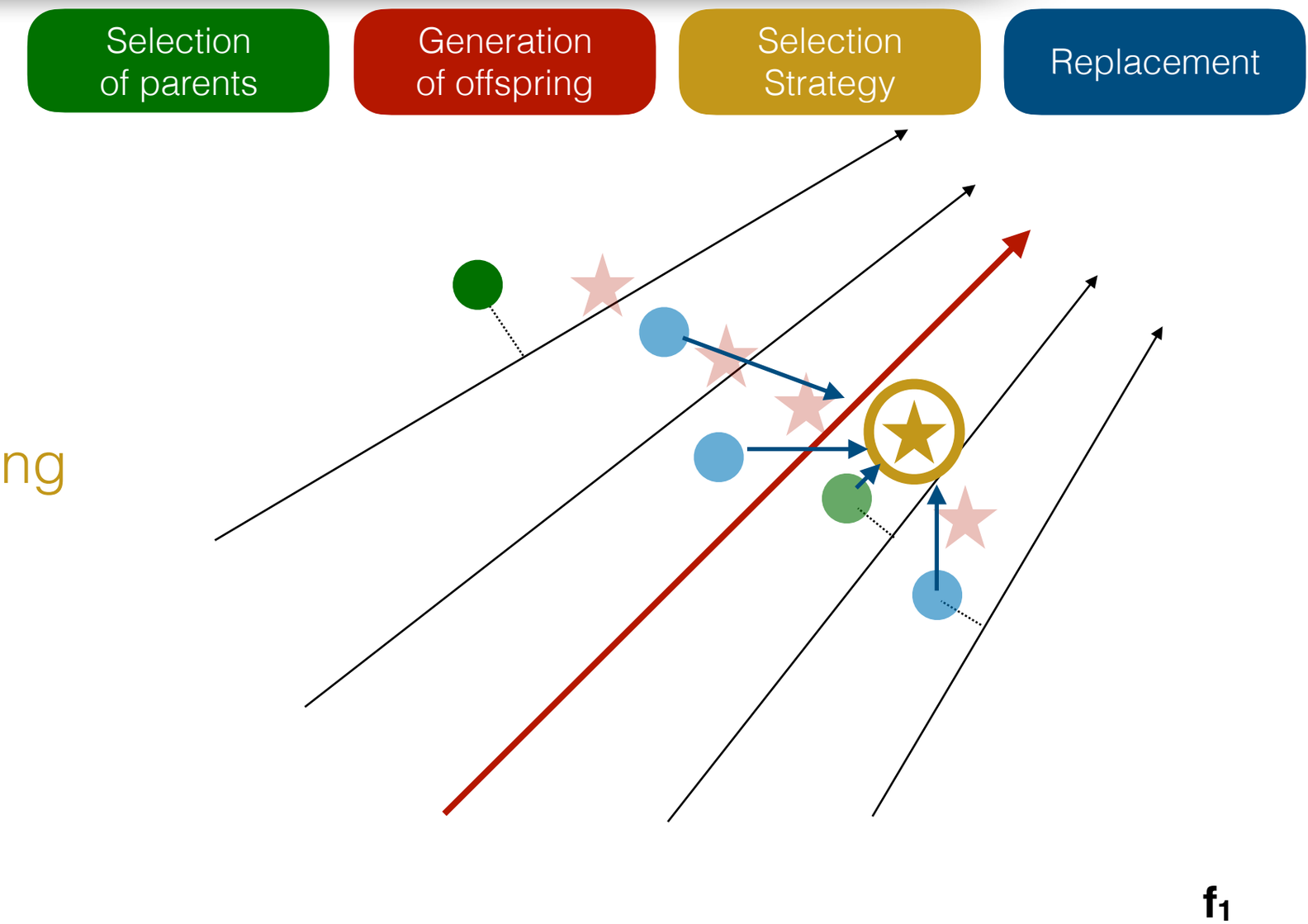

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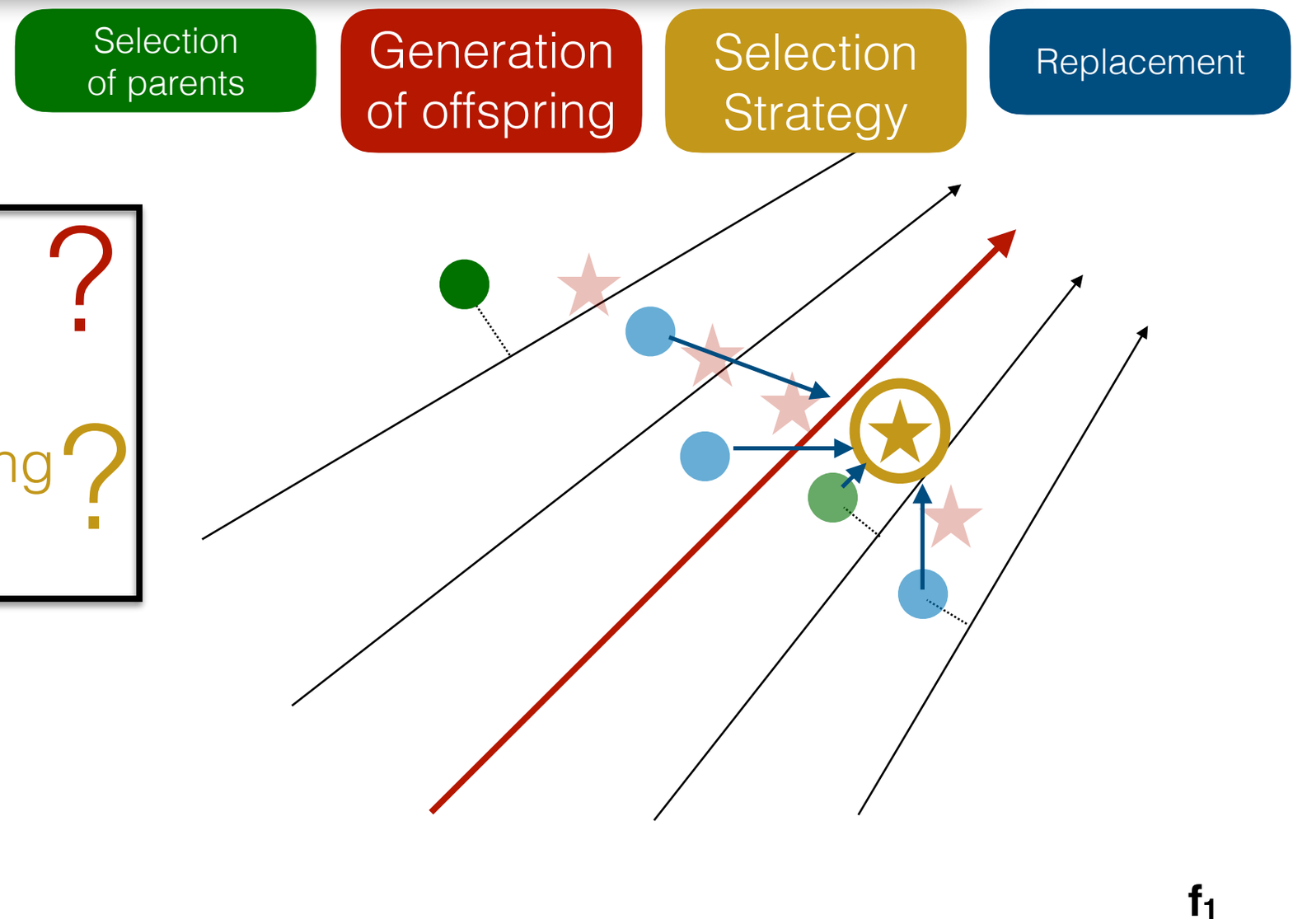
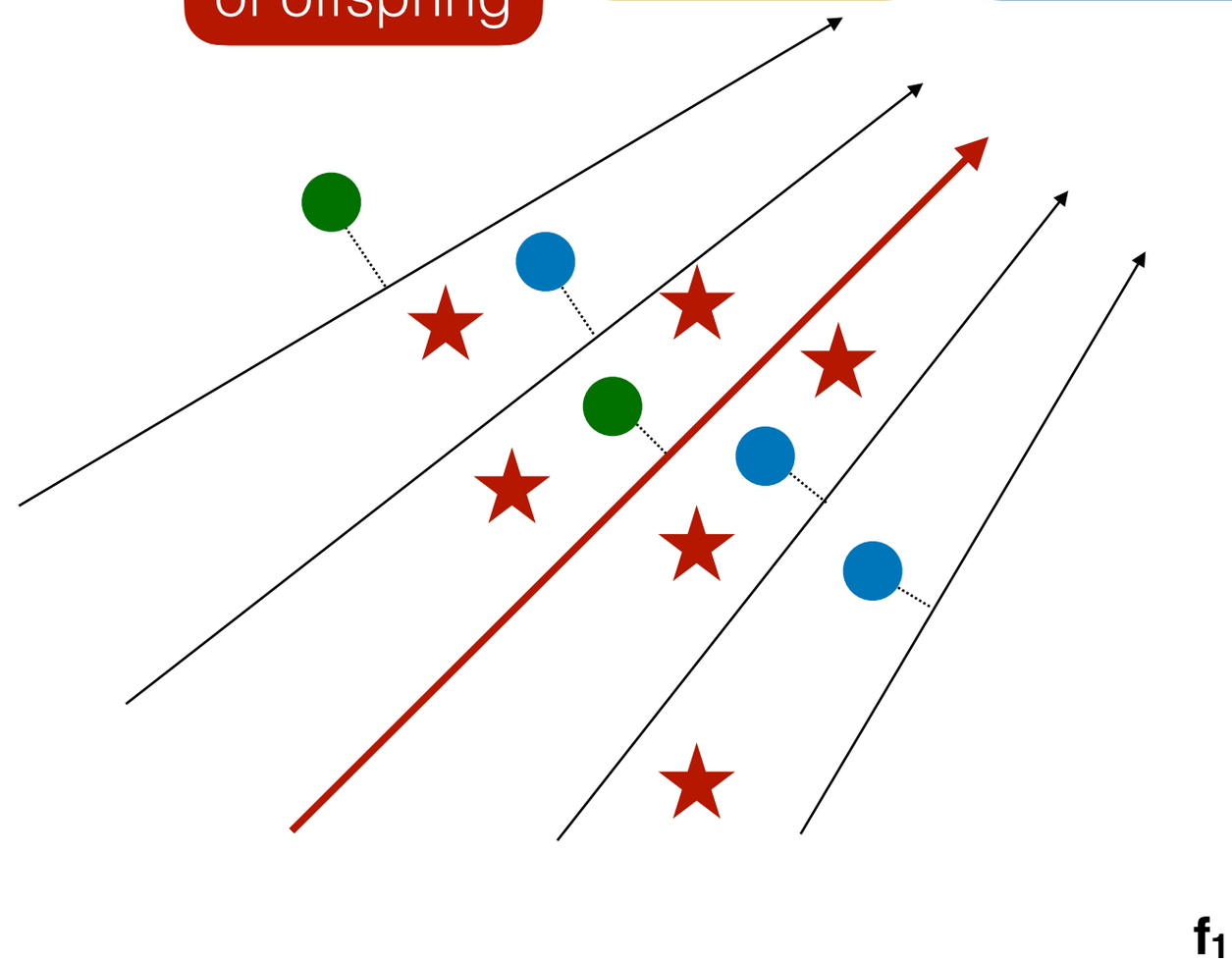


The S-CMO Framework

Surrogate-assisted Combinatorial Multi-objective Optimization Framework

Selection of parents | Generation of offspring | Selection Strategy | Replacement

- Generate **Offspring In *S-CMO***
  - **<u>Filtering</u>**
    - Generate λ solutions with variation operators
    - Evaluated with $\tilde{F}(x)$

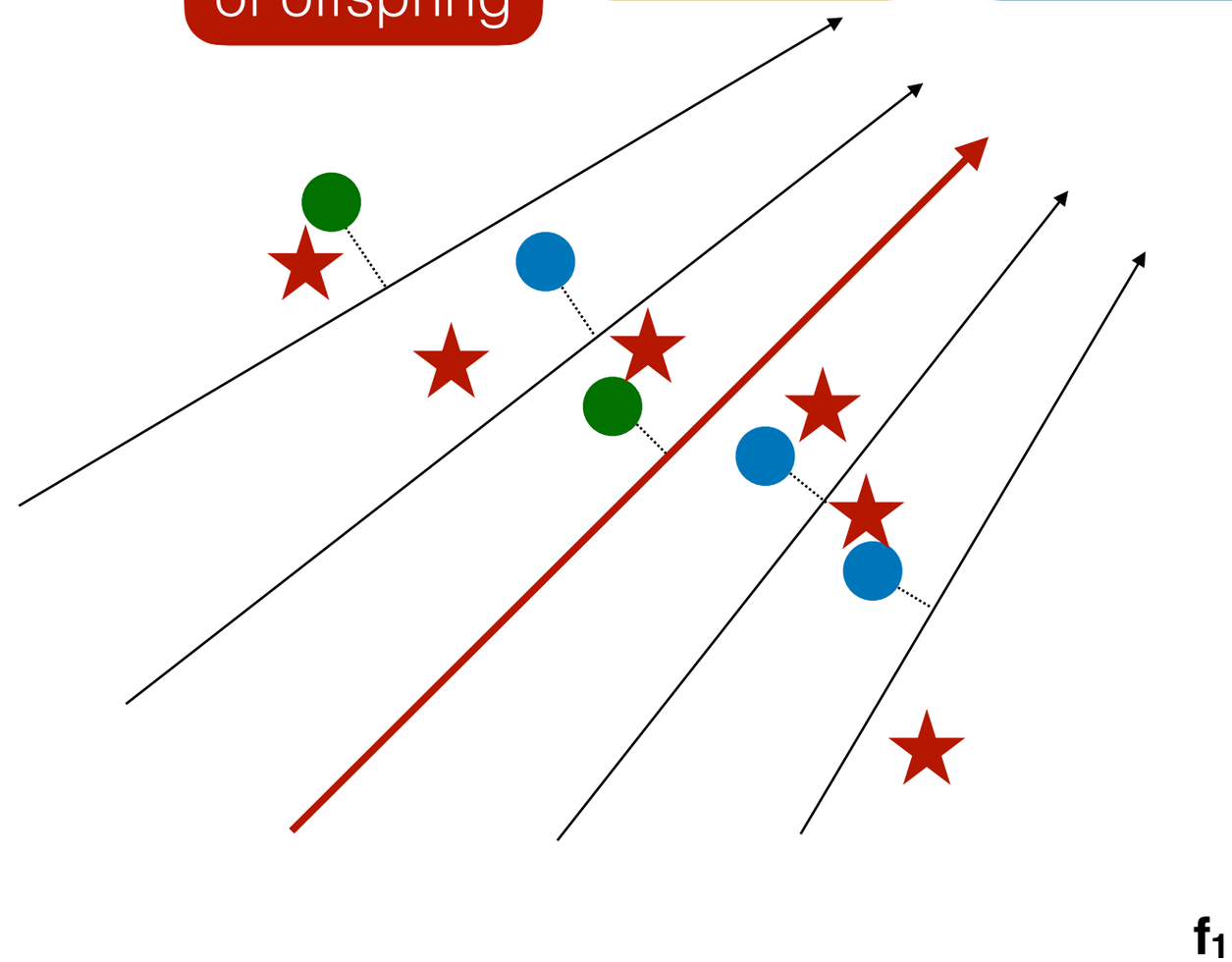


The S-CMO Framework

Surrogate-assisted Combinatorial Multi-objective Optimization Framework

Selection of parents | Generation of offspring | Selection Strategy | Replacement

- Generate **Offspring In *S-CMO***
  - Filtering
    - Generate λ solutions with variation operators
    - Evaluated with $\tilde{F}(x)$
  - **<u>Substitution</u>**
    - Use an optimization engine with the $\tilde{F}(x)$



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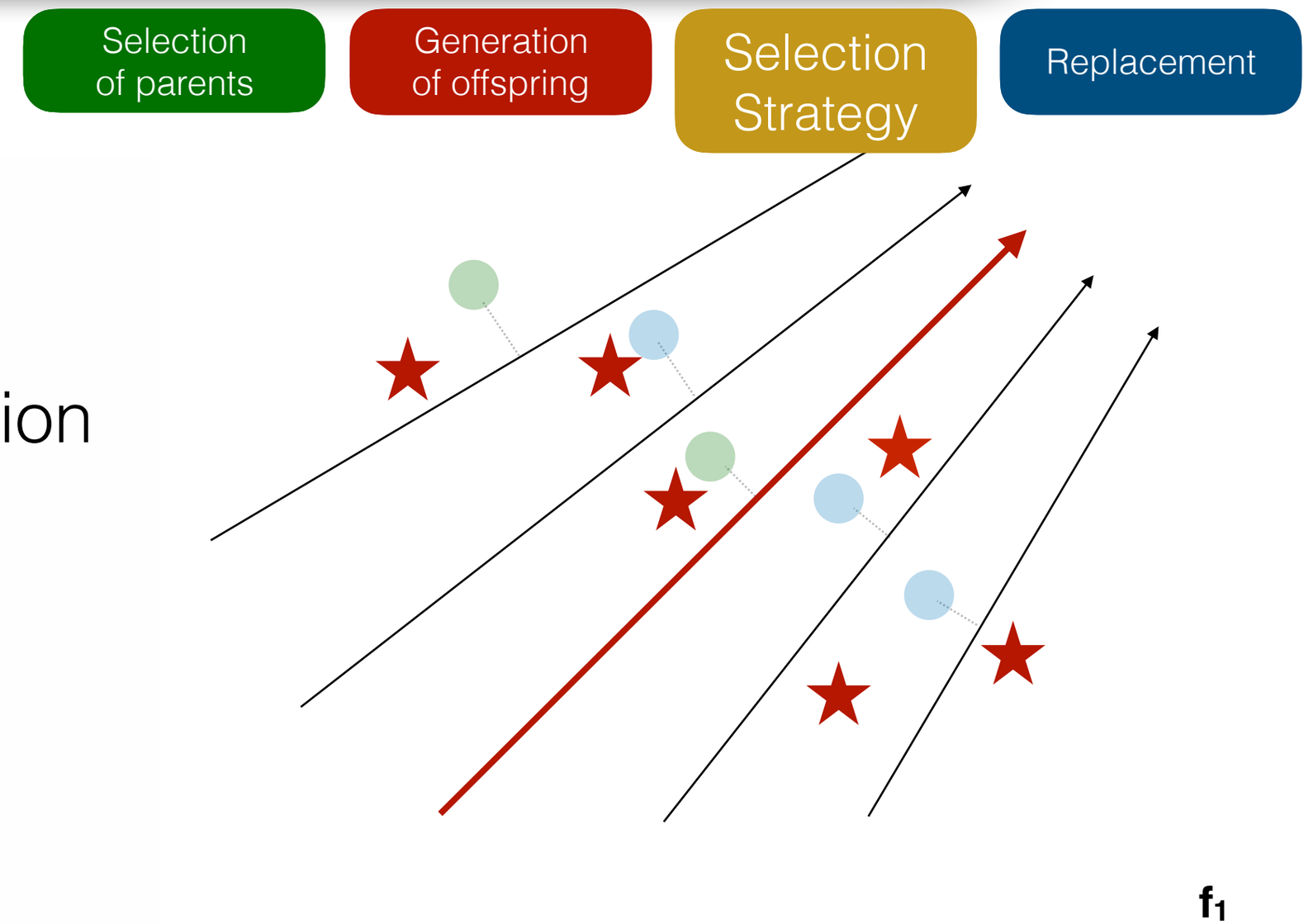
Surrogate-assisted Combinatorial Multi-objective Optimization Framework

- **Selection strategy**

We want select the best offspring without evaluation



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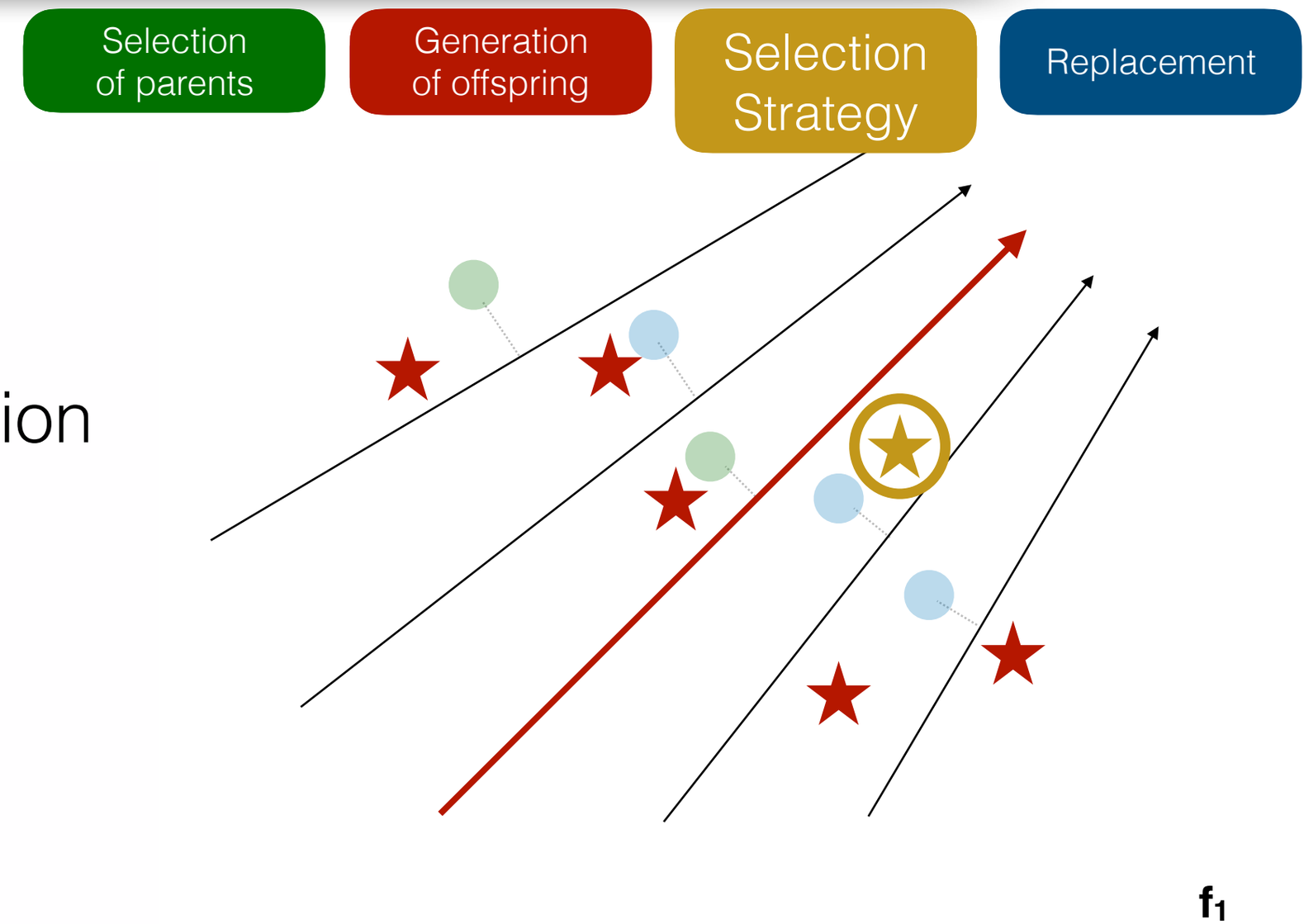

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- **Selection strategy**
  - **<u>Local</u>**
    - The best g-value
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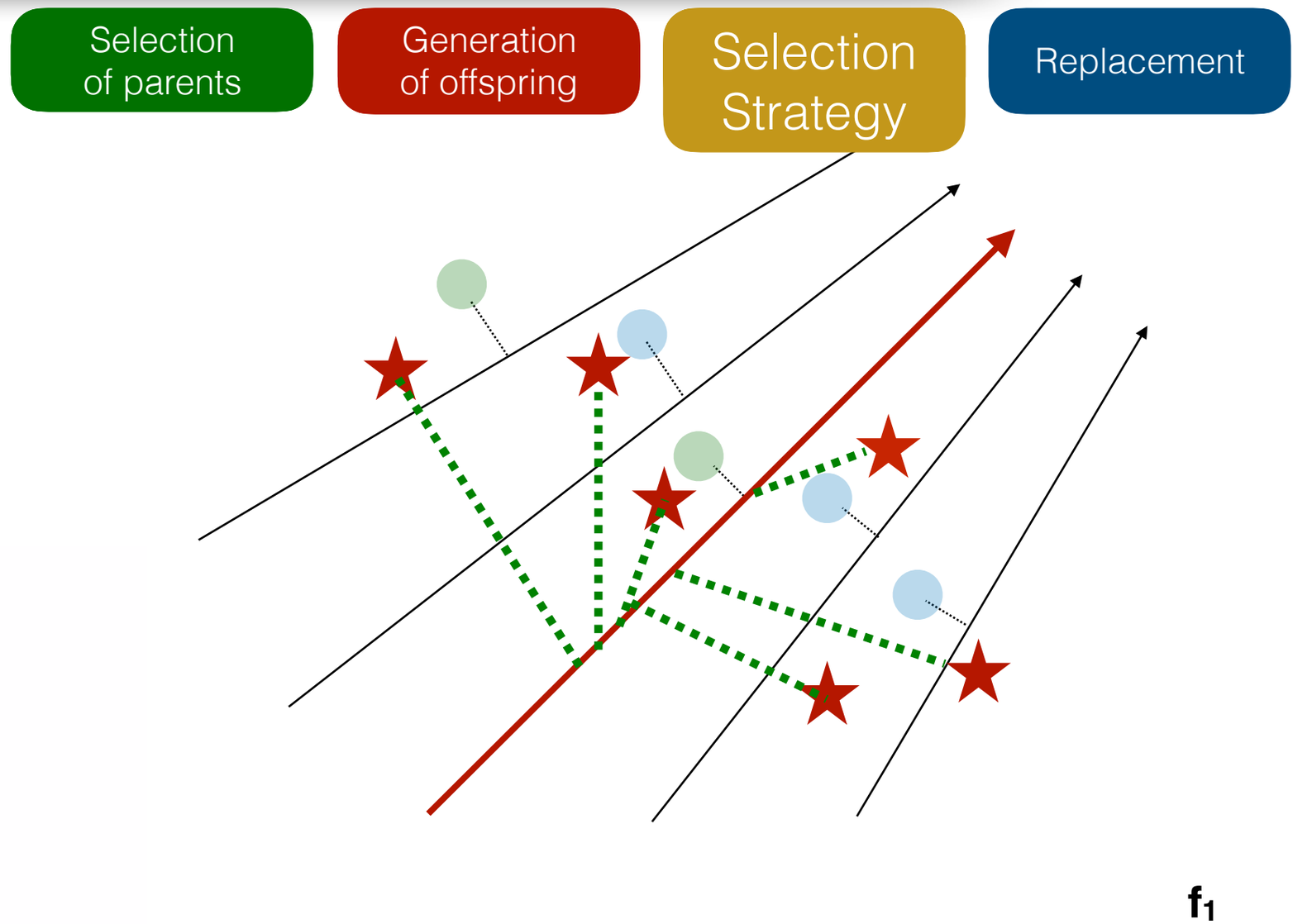

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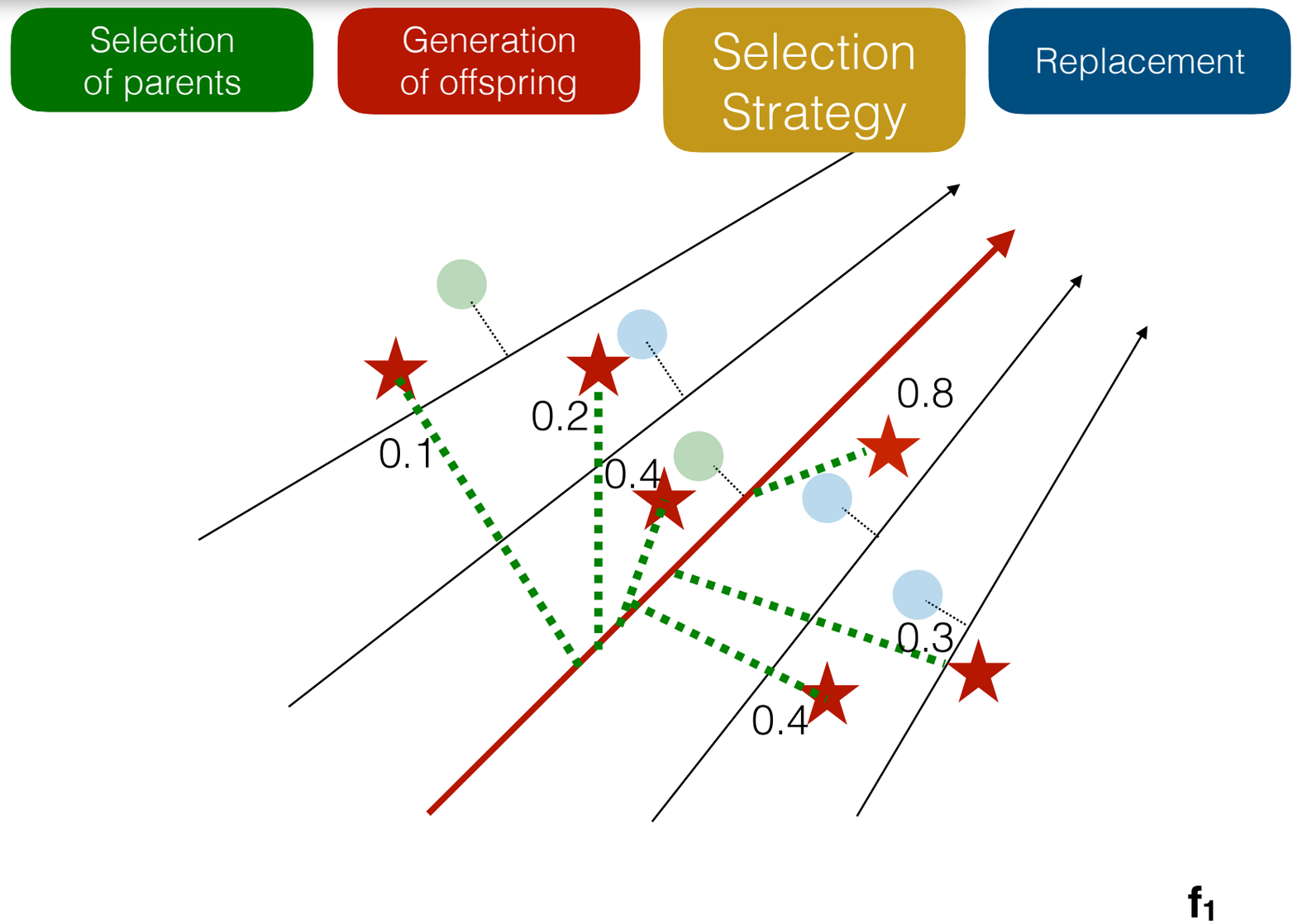

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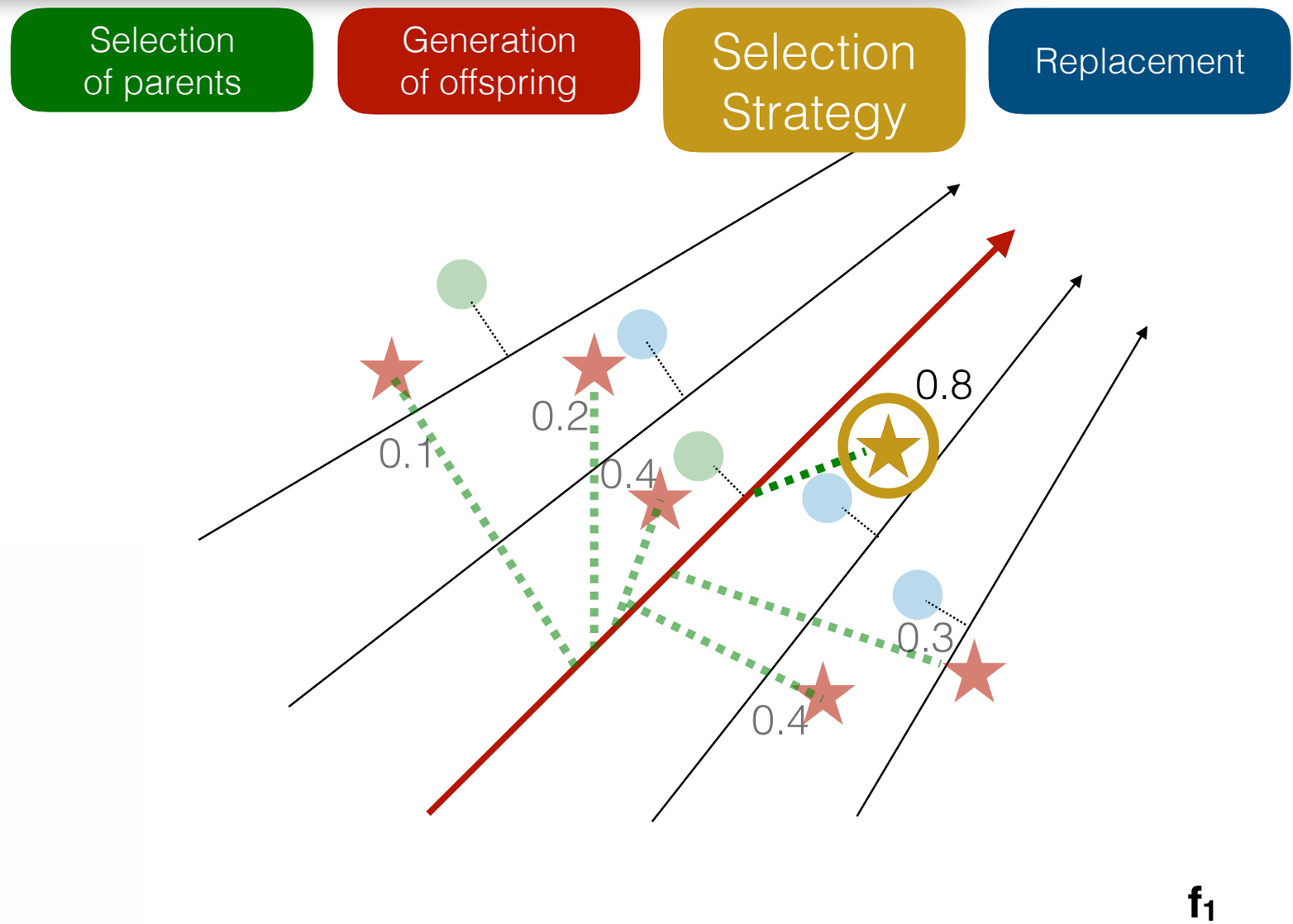

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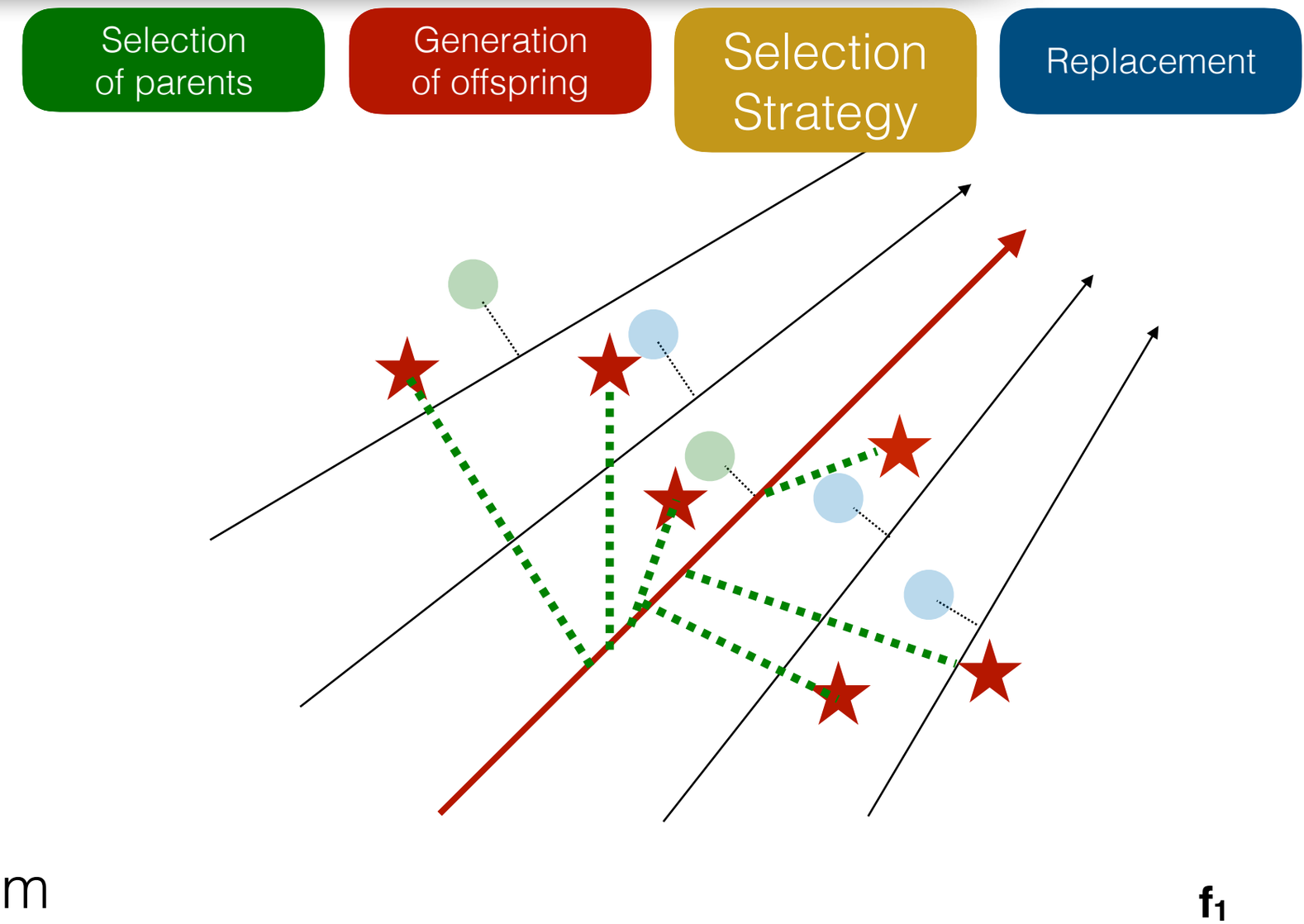

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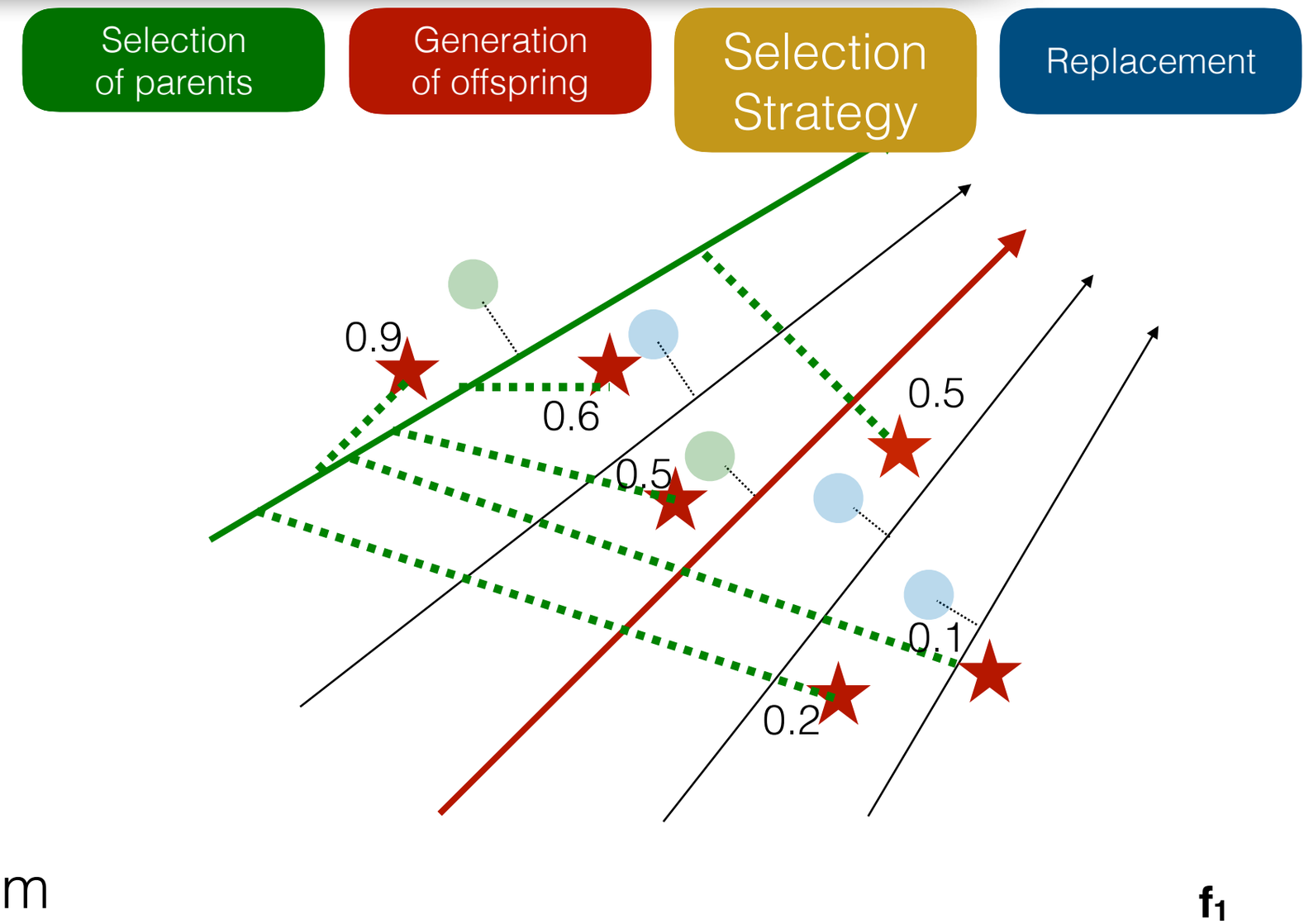

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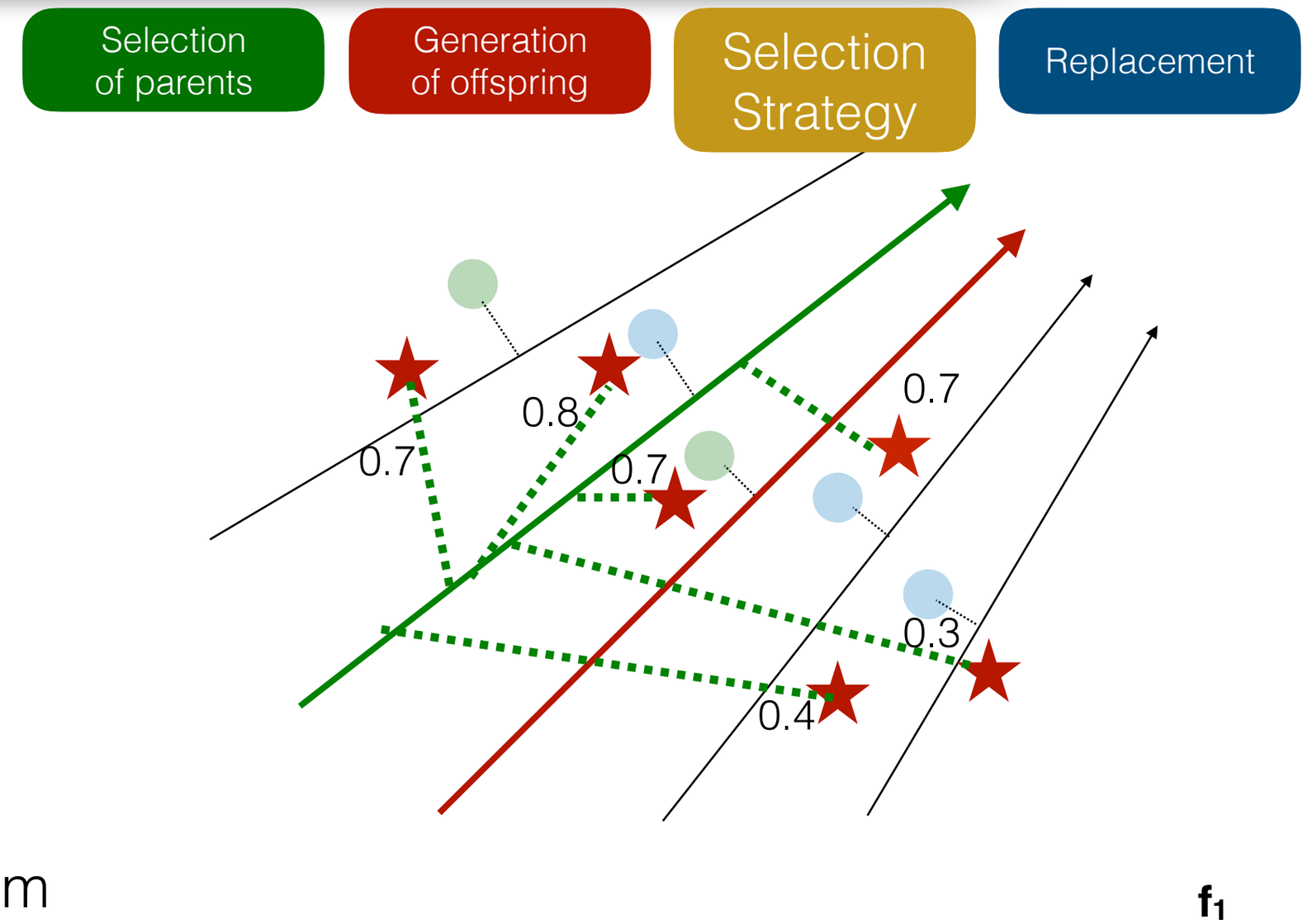

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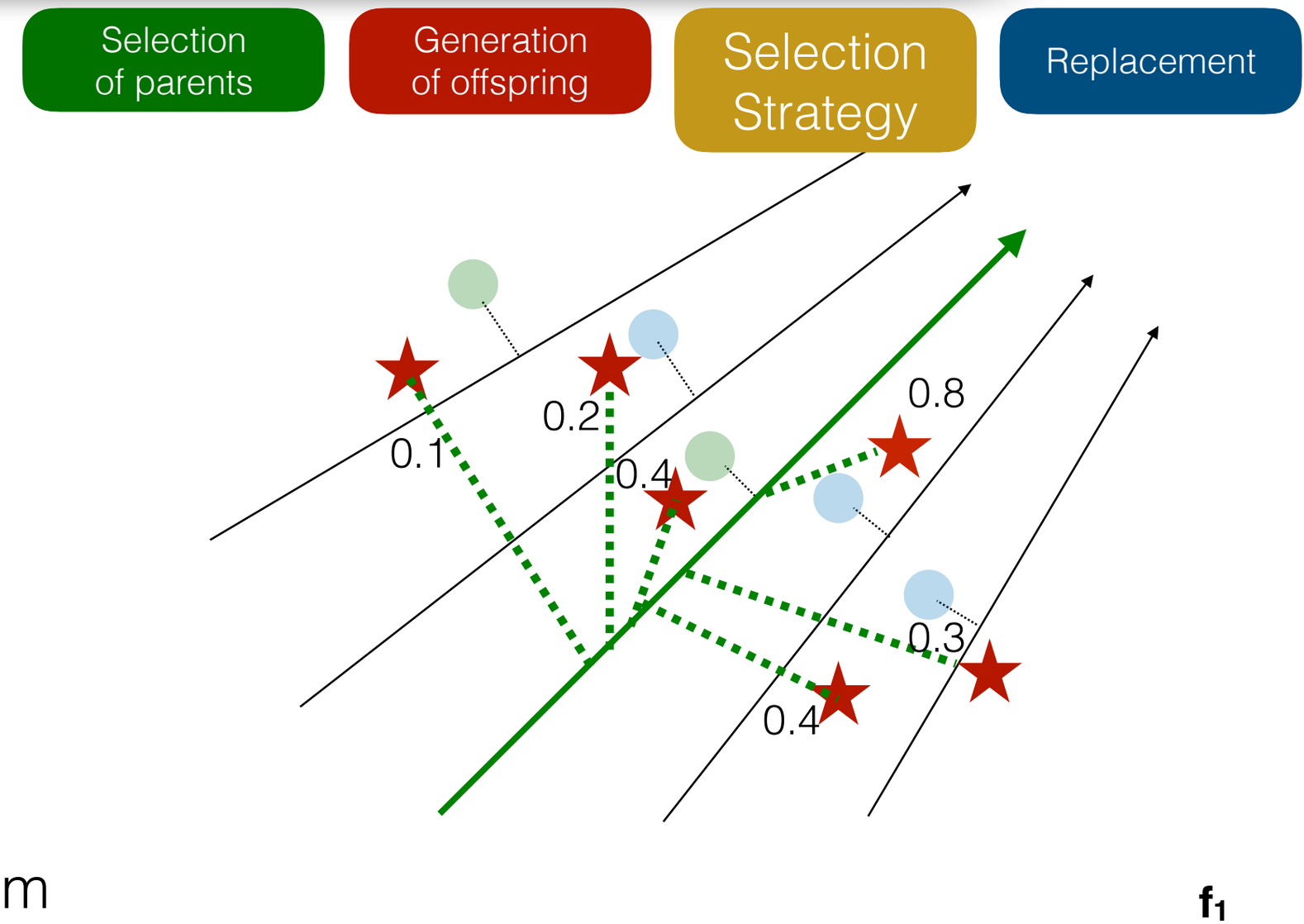

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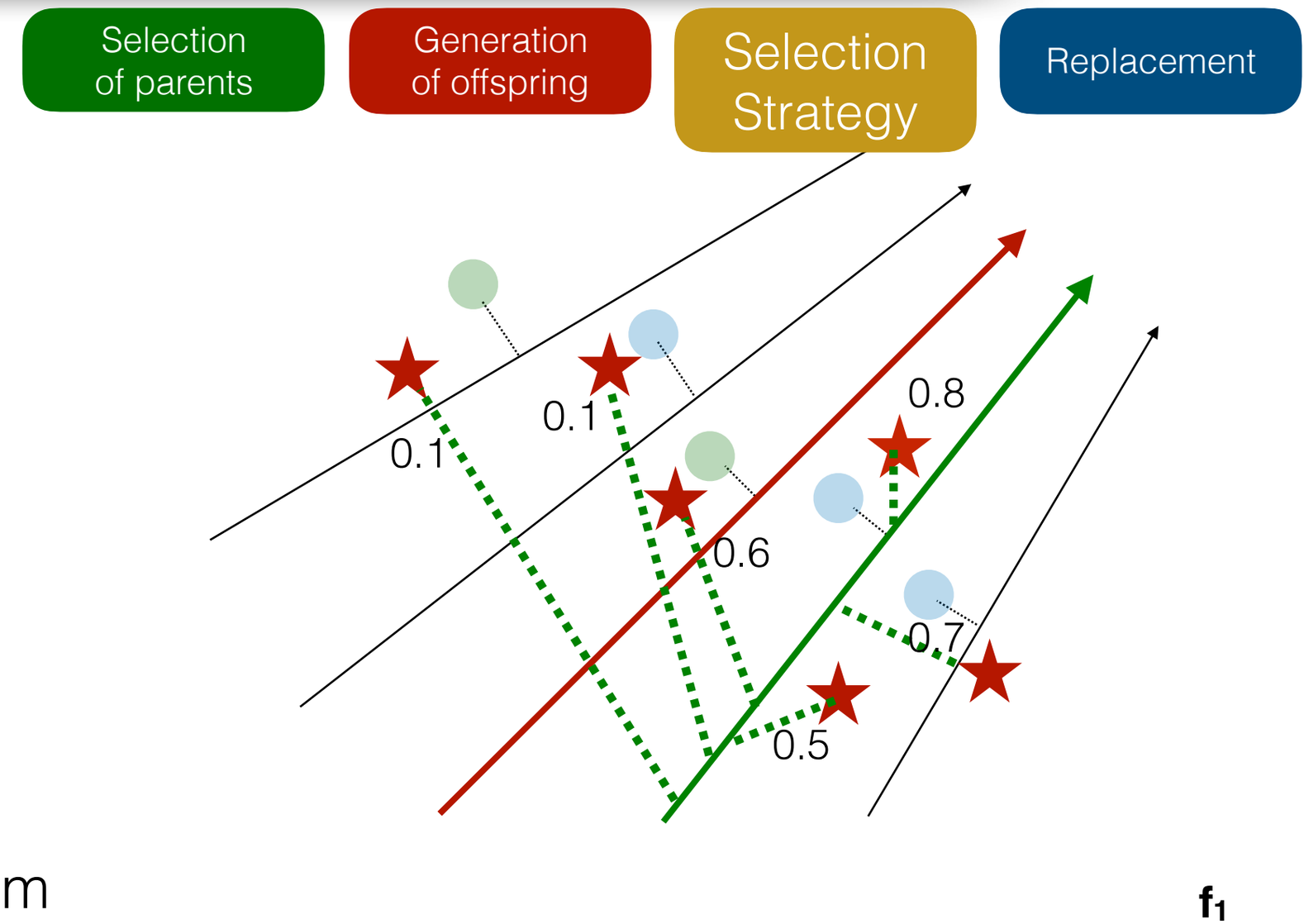

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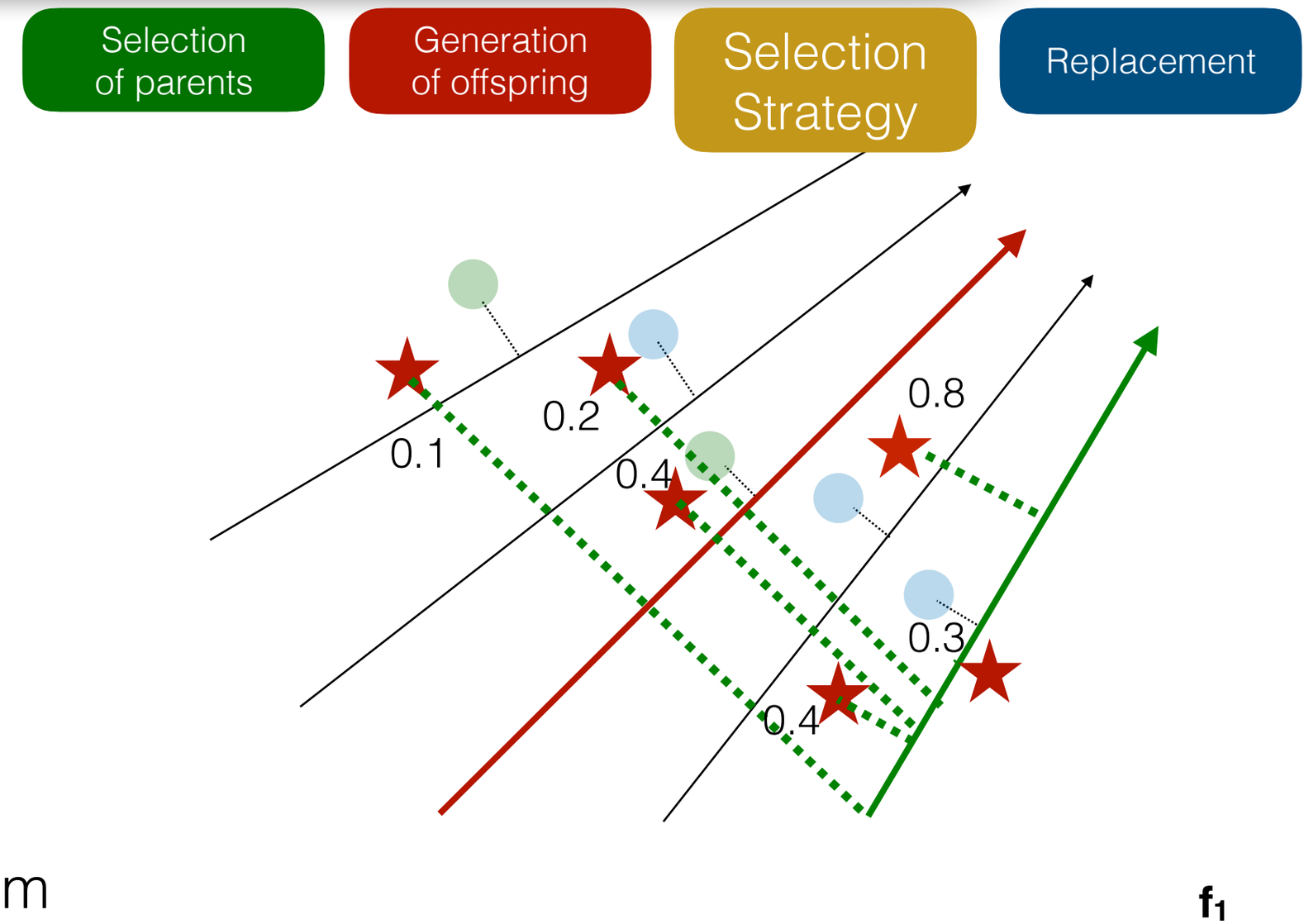

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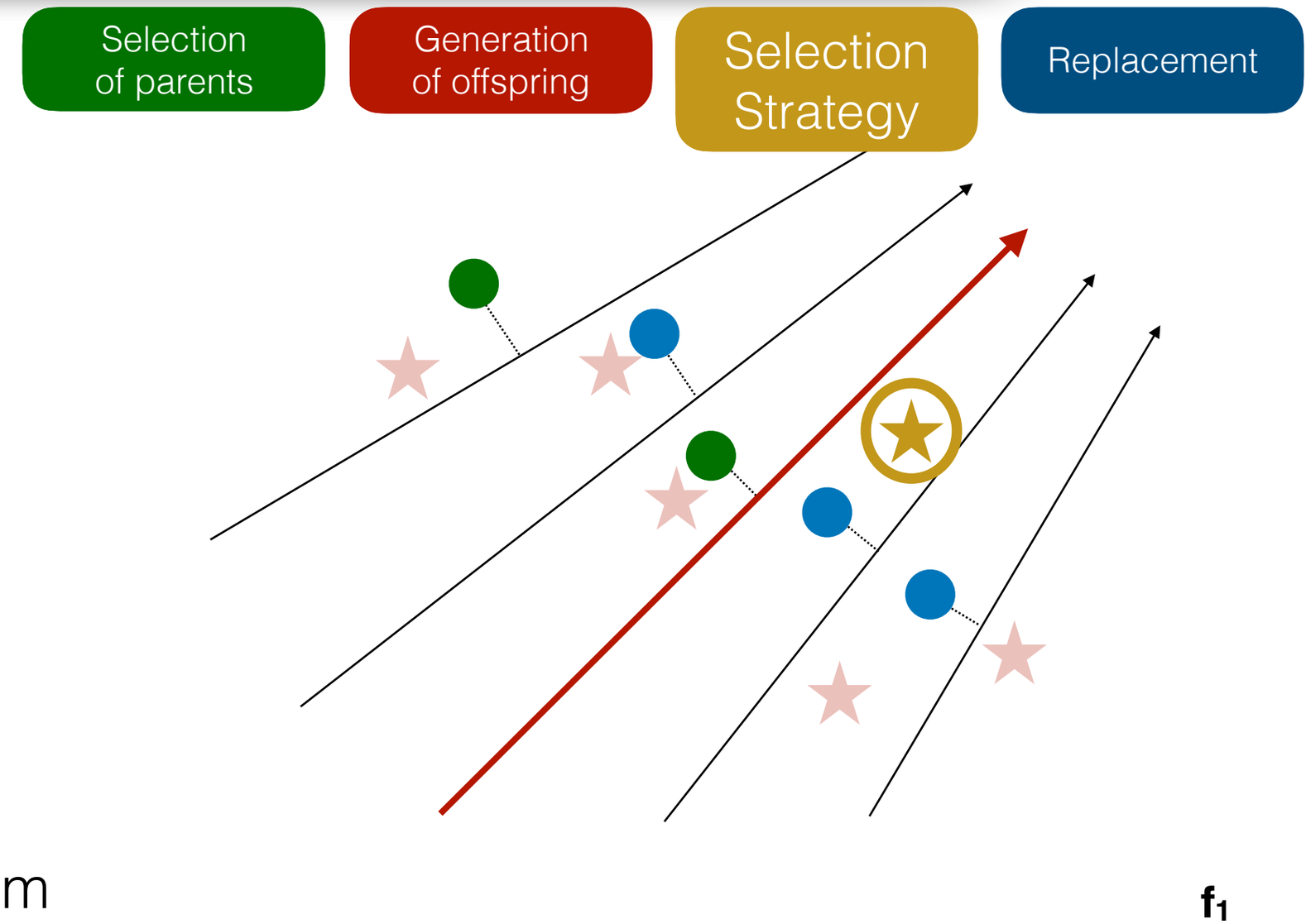
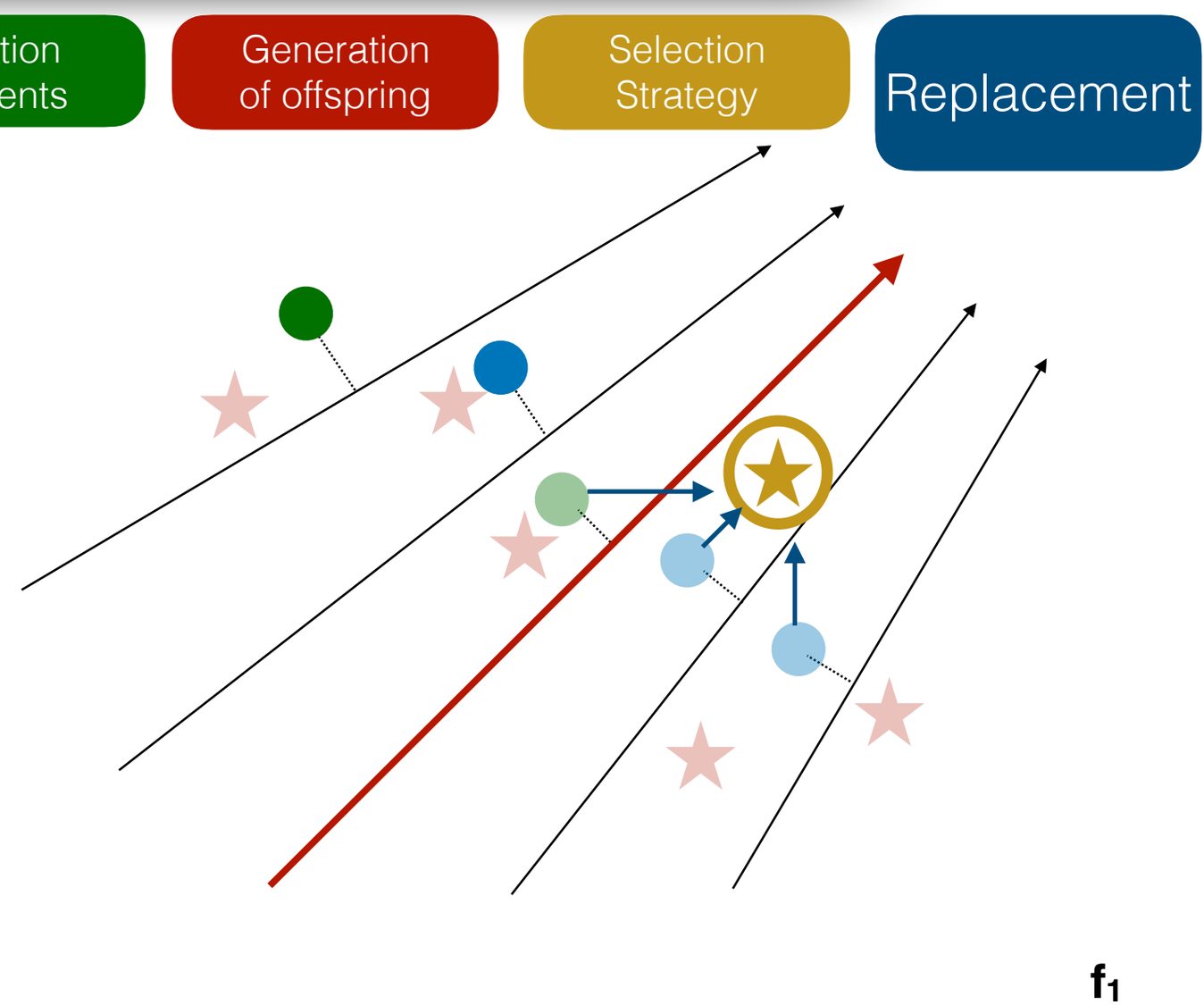


The S-CMO Framework

Surrogate-assisted Combinatorial Multi-objective Optimization Framework

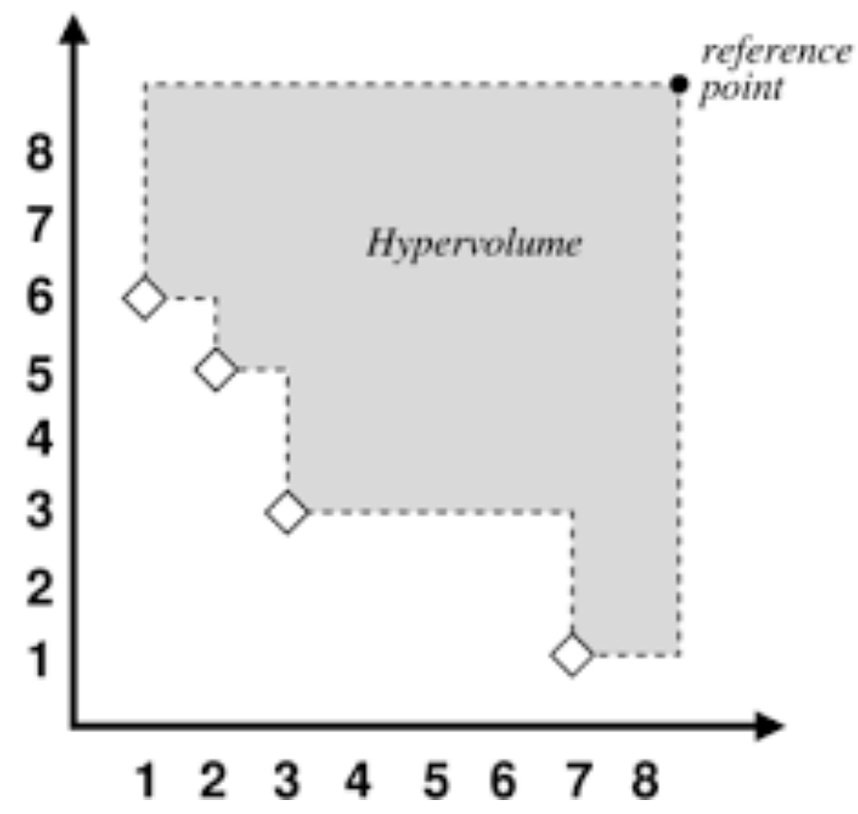
- **Replacement**

Same as in MOEA/D by using the aggregation value



Experimental Setting

- Benchmark : **multi-objective NK-landscapes**
  - combinatorial problem
  - representation = bit-strings
  - problem size n = {25, 50} (decision space dimension)
  - k={0, 1, 2} epistatic interactions to manage the ruggedness of the problem
  - m= 2 objectives
- Walsh Order : {1, 2, 3} / Optimal Order = k+1
- Lasso Regression
- Indicator : **hypervolume**
- Number of runs : **10**
- Number of evaluation : **1500**



Impact of the selection strategy

Local or Global ?

			$n = 25$			$n = 50$			
			$k = 0$	$k = 1$	$k = 2$	$k = 0$	$k = 1$	$k = 2$	avg. rank
budget = 500	MOEA/D		$1_{(7.71)}$	$2_{(12.49)}$	$2_{(10.47)}$	$2_{(5.59)}$	$3_{(5.9)}$	$1_{(6.81)}$	1.83
	Filter	Local	$1_{(7.83)}$	$3_{(12.74)}$	$1_{(10.71)}$	$2_{(5.58)}$	$3_{(6)}$	$1_{(6.8)}$	1.83
	Filter	Global	$\mathbf{0}_{(\underline{8.04})}$	$\mathbf{0}_{(\underline{13.36})}$	$1_{(11.04)}$	$1_{(5.95)}$	$1_{(6.41)}$	$1_{(7.1)}$	0.66
	Substitute	Local	$3_{(7.38)}$	$\mathbf{0}_{(13.18)}$	$1_{(10.82)}$	$2_{(5.75)}$	$1_{(6.51)}$	$1_{(7.15)}$	1.33
	Substitute	Global	$1_{(7.47)}$	$\mathbf{0}_{(13.35)}$	$\mathbf{0}_{(\underline{11.62})}$	$\mathbf{0}_{(\underline{6.65})}$	$\mathbf{0}_{(\underline{7.16})}$	$\mathbf{0}_{(\underline{7.93})}$	0.16
budget = 1 500	MOEA/D		$2_{(8.07)}$	$2_{(13.39)}$	$1_{(11.58)}$	$2_{(6.27)}$	$3_{(6.73)}$	$2_{(7.88)}$	2.00
	Filter	Local	$2_{(8.12)}$	$2_{(13.32)}$	$2_{(11.39)}$	$2_{(6.16)}$	$3_{(6.68)}$	$3_{(7.72)}$	2.33
	Filter	Global	$\mathbf{0}_{(8.3)}$	$\mathbf{0}_{(\underline{1.36})}$	$1_{(1.18)}$	$1_{(6.51)}$	$1_{(7.06)}$	$1_{(8.11)}$	0.66
	Substitute	Local	$2_{(8.06)}$	$\mathbf{0}_{(13.58)}$	$1_{(11.71)}$	$2_{(6.29)}$	$1_{(6.99)}$	$1_{(8.16)}$	1.16
	Substitute	Global	$\mathbf{0}_{(\underline{8.31})}$	$2_{(13.44)}$	$\mathbf{0}_{(\underline{12.32})}$	$\mathbf{0}_{(\underline{6.85})}$	$\mathbf{0}_{(\underline{7.38})}$	$\mathbf{0}_{(\underline{8.54})}$	0.33

Impact of the selection strategy

Local or Global ?

			$n = 25$			$n = 50$			
			$k = 0$	$k = 1$	$k = 2$	$k = 0$	$k = 1$	$k = 2$	avg. rank
budget = 500	MOEA/D		$\boxed{1}_{(7.71)}$	$\boxed{2}_{(12.49)}$	$\boxed{2}_{(10.47)}$	$\boxed{2}_{(5.59)}$	$\boxed{3}_{(5.9)}$	$\boxed{1}_{(6.81)}$	1.83
	Filter	Local	$1_{(7.83)}$	$3_{(12.74)}$	$1_{(10.71)}$	$2_{(5.58)}$	$3_{(6)}$	$1_{(6.8)}$	1.83
	Filter	Global	$\mathbf{0}_{(\underline{8.04})}$	$\mathbf{0}_{(\underline{13.36})}$	$1_{(11.04)}$	$1_{(5.95)}$	$1_{(6.41)}$	$1_{(7.1)}$	0.66
	Substitute	Local	$3_{(7.38)}$	$\mathbf{0}_{(13.18)}$	$1_{(10.82)}$	$2_{(5.75)}$	$1_{(6.51)}$	$1_{(7.15)}$	1.33
	Substitute	Global	$1_{(7.47)}$	$\mathbf{0}_{(13.35)}$	$\mathbf{0}_{(\underline{11.62})}$	$\mathbf{0}_{(\underline{6.65})}$	$\mathbf{0}_{(\underline{7.16})}$	$\mathbf{0}_{(\underline{7.93})}$	0.16
budget = 1 500	MOEA/D		$2_{(8.07)}$	$2_{(13.39)}$	$1_{(11.58)}$	$2_{(6.27)}$	$3_{(6.73)}$	$2_{(7.88)}$	2.00
	Filter	Local	$2_{(8.12)}$	$2_{(13.32)}$	$2_{(11.39)}$	$2_{(6.16)}$	$3_{(6.68)}$	$3_{(7.72)}$	2.33
	Filter	Global	$\mathbf{0}_{(8.3)}$	$\mathbf{0}_{(\underline{1.36})}$	$1_{(1.18)}$	$1_{(6.51)}$	$1_{(7.06)}$	$1_{(8.11)}$	0.66
	Substitute	Local	$2_{(8.06)}$	$\mathbf{0}_{(13.58)}$	$1_{(11.71)}$	$2_{(6.29)}$	$1_{(6.99)}$	$1_{(8.16)}$	1.16
	Substitute	Global	$\mathbf{0}_{(\underline{8.31})}$	$2_{(13.44)}$	$\mathbf{0}_{(\underline{12.32})}$	$\mathbf{0}_{(\underline{6.85})}$	$\mathbf{0}_{(\underline{7.38})}$	$\mathbf{0}_{(\underline{8.54})}$	0.33

Impact of the selection strategy

Local or Global ?

			$n = 25$			$n = 50$			
			$k = 0$	$k = 1$	$k = 2$	$k = 0$	$k = 1$	$k = 2$	avg. rank
budget = 500	MOEA/D		1 (7.71)	2 (12.49)	2 (10.47)	2 (5.59)	3 (5.9)	1 (6.81)	1.83
	Filter	Local	1 (7.83)	3 (12.74)	1 (10.71)	2 (5.58)	3 (6)	1 (6.8)	1.83
	Filter	Global	**0** (8.04)	**0** (13.36)	1 (11.04)	1 (5.95)	1 (6.41)	1 (7.1)	0.66
	Substitute	Local	3 (7.38)	**0** (13.18)	1 (10.82)	2 (5.75)	1 (6.51)	1 (7.15)	1.33
	Substitute	Global	1 (7.47)	**0** (13.35)	**0** (11.62)	**0** (6.65)	**0** (7.16)	**0** (7.93)	0.16
budget = 1 500	MOEA/D		2 (8.07)	2 (13.39)	1 (11.58)	2 (6.27)	3 (6.73)	2 (7.88)	2.00
	Filter	Local	2 (8.12)	2 (13.32)	2 (11.39)	2 (6.16)	3 (6.68)	3 (7.72)	2.33
	Filter	Global	**0** (8.3)	**0** (1.36)	1 (1.18)	1 (6.51)	1 (7.06)	1 (8.11)	0.66
	Substitute	Local	2 (8.06)	**0** (13.58)	1 (11.71)	2 (6.29)	1 (6.99)	1 (8.16)	1.16
	Substitute	Global	**0** (8.31)	2 (13.44)	**0** (12.32)	**0** (6.85)	**0** (7.38)	**0** (8.54)	0.33

Impact of the selection strategy

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			$n = 25$			$n = 50$			
			$k = 0$	$k = 1$	$k = 2$	$k = 0$	$k = 1$	$k = 2$	avg. rank
budget = 500	MOEA/D		$1_{(7.71)}$	$2_{(12.49)}$	$2_{(10.47)}$	$2_{(5.59)}$	$3_{(5.9)}$	$1_{(6.81)}$	1.83
	Filter	Local	$1_{(7.83)}$	$3_{(12.74)}$	$1_{(10.71)}$	$2_{(5.58)}$	$3_{(6)}$	$1_{(6.8)}$	1.83
	Filter	Global	$\mathbf{0}_{(\underline{8.04})}$	$\mathbf{0}_{(\underline{13.36})}$	$1_{(11.04)}$	$1_{(5.95)}$	$1_{(6.41)}$	$1_{(7.1)}$	0.66
	Substitute	Local	$3_{(7.38)}$	$\mathbf{0}_{(13.18)}$	$1_{(10.82)}$	$2_{(5.75)}$	$1_{(6.51)}$	$1_{(7.15)}$	1.33
	Substitute	Global	$1_{(7.47)}$	$\mathbf{0}_{(13.35)}$	$\mathbf{0}_{(\underline{11.62})}$	$\mathbf{0}_{(\underline{6.65})}$	$\mathbf{0}_{(\underline{7.16})}$	$\mathbf{0}_{(\underline{7.93})}$	0.16
budget = 1 500	MOEA/D		$2_{(8.07)}$	$2_{(13.39)}$	$1_{(11.58)}$	$2_{(6.27)}$	$3_{(6.73)}$	$2_{(7.88)}$	2.00
	Filter	Local	$2_{(8.12)}$	$2_{(13.32)}$	$2_{(11.39)}$	$2_{(6.16)}$	$3_{(6.68)}$	$3_{(7.72)}$	2.33
	Filter	Global	$\mathbf{0}_{(8.3)}$	$\mathbf{0}_{(\underline{1.36})}$	$1_{(1.18)}$	$1_{(6.51)}$	$1_{(7.06)}$	$1_{(8.11)}$	0.66
	Substitute	Local	$2_{(8.06)}$	$\mathbf{0}_{(13.58)}$	$1_{(11.71)}$	$2_{(6.29)}$	$1_{(6.99)}$	$1_{(8.16)}$	1.16
	Substitute	Global	$\mathbf{0}_{(\underline{8.31})}$	$2_{(13.44)}$	$\mathbf{0}_{(\underline{12.32})}$	$\mathbf{0}_{(\underline{6.85})}$	$\mathbf{0}_{(\underline{7.38})}$	$\mathbf{0}_{(\underline{8.54})}$	0.33

Impact of the selection strategy

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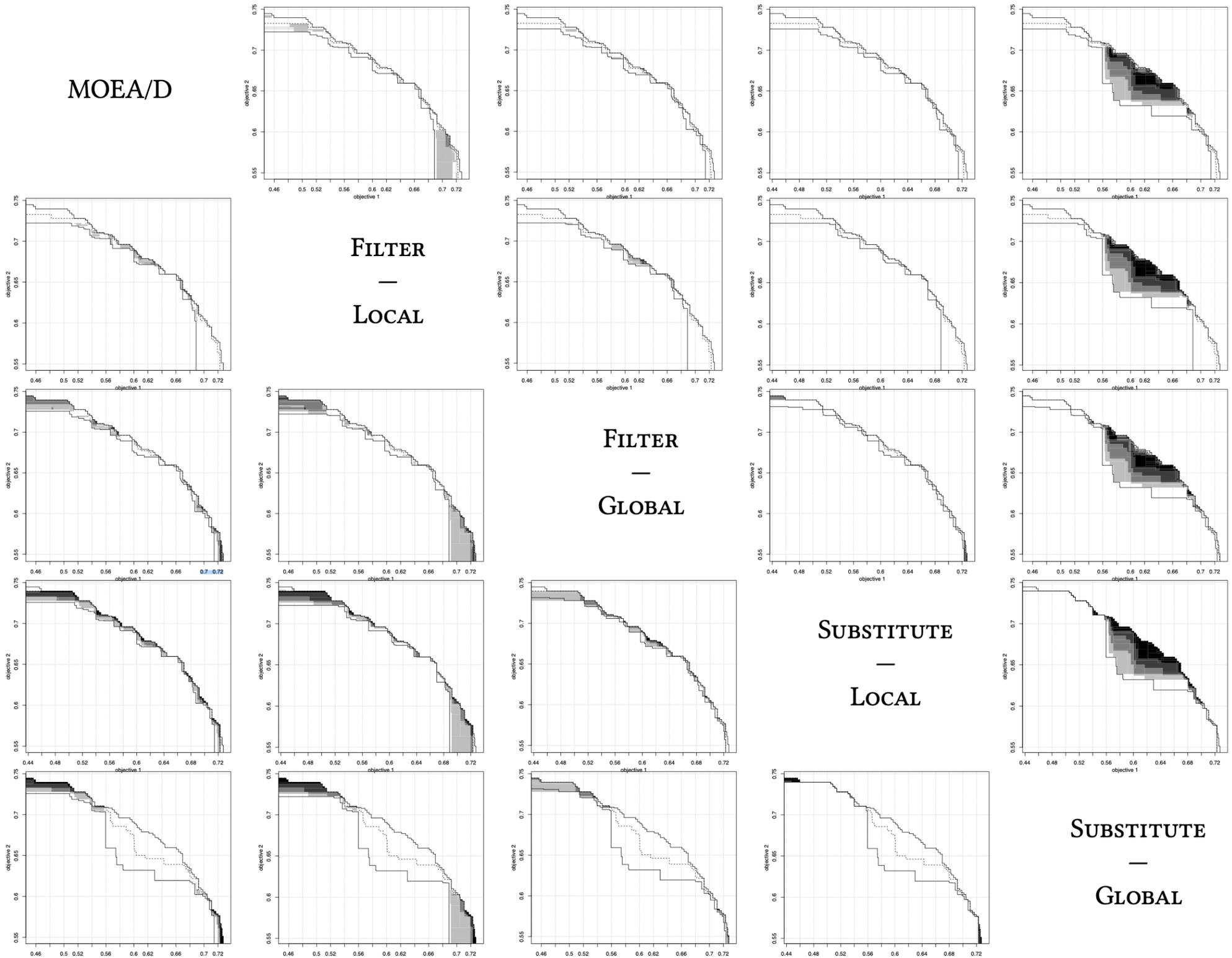
			$n = 25$			$n = 50$			
			$k = 0$	$k = 1$	$k = 2$	$k = 0$	$k = 1$	$k = 2$	avg. rank
budget = 500	MOEA/D		$1_{(7.71)}$	$2_{(12.49)}$	$2_{(10.47)}$	$2_{(5.59)}$	$3_{(5.9)}$	$1_{(6.81)}$	1.83
	Filter	Local	$1_{(7.83)}$	$3_{(12.74)}$	$1_{(10.71)}$	$2_{(5.58)}$	$3_{(6)}$	$1_{(6.8)}$	1.83
	Filter	Global	$\mathbf{0}_{(\underline{8.04})}$	$\mathbf{0}_{(\underline{13.36})}$	$1_{(11.04)}$	$1_{(5.95)}$	$1_{(6.41)}$	$1_{(7.1)}$	0.66
	Substitute	Local	$3_{(7.38)}$	$\mathbf{0}_{(13.18)}$	$1_{(10.82)}$	$2_{(5.75)}$	$1_{(6.51)}$	$1_{(7.15)}$	1.33
	Substitute	Global	$1_{(7.47)}$	$\mathbf{0}_{(13.35)}$	$\mathbf{0}_{(\underline{11.62})}$	$\mathbf{0}_{(\underline{6.65})}$	$\mathbf{0}_{(\underline{7.16})}$	$\mathbf{0}_{(\underline{7.93})}$	0.16
budget = 1 500	MOEA/D		$2_{(8.07)}$	$2_{(13.39)}$	$1_{(11.58)}$	$2_{(6.27)}$	$3_{(6.73)}$	$2_{(7.88)}$	2.00
	Filter	Local	$2_{(8.12)}$	$2_{(13.32)}$	$2_{(11.39)}$	$2_{(6.16)}$	$3_{(6.68)}$	$3_{(7.72)}$	2.33
	Filter	Global	$\mathbf{0}_{(8.3)}$	$\mathbf{0}_{(\underline{1.36})}$	$1_{(1.18)}$	$1_{(6.51)}$	$1_{(7.06)}$	$1_{(8.11)}$	0.66
	Substitute	Local	$2_{(8.06)}$	$\mathbf{0}_{(13.58)}$	$1_{(11.71)}$	$2_{(6.29)}$	$1_{(6.99)}$	$1_{(8.16)}$	1.16
	Substitute	Global	$\mathbf{0}_{(\underline{8.31})}$	$2_{(13.44)}$	$\mathbf{0}_{(\underline{12.32})}$	$\mathbf{0}_{(\underline{6.85})}$	$\mathbf{0}_{(\underline{7.38})}$	$\mathbf{0}_{(\underline{8.54})}$	0.33

Local Strategy

Global Strategy

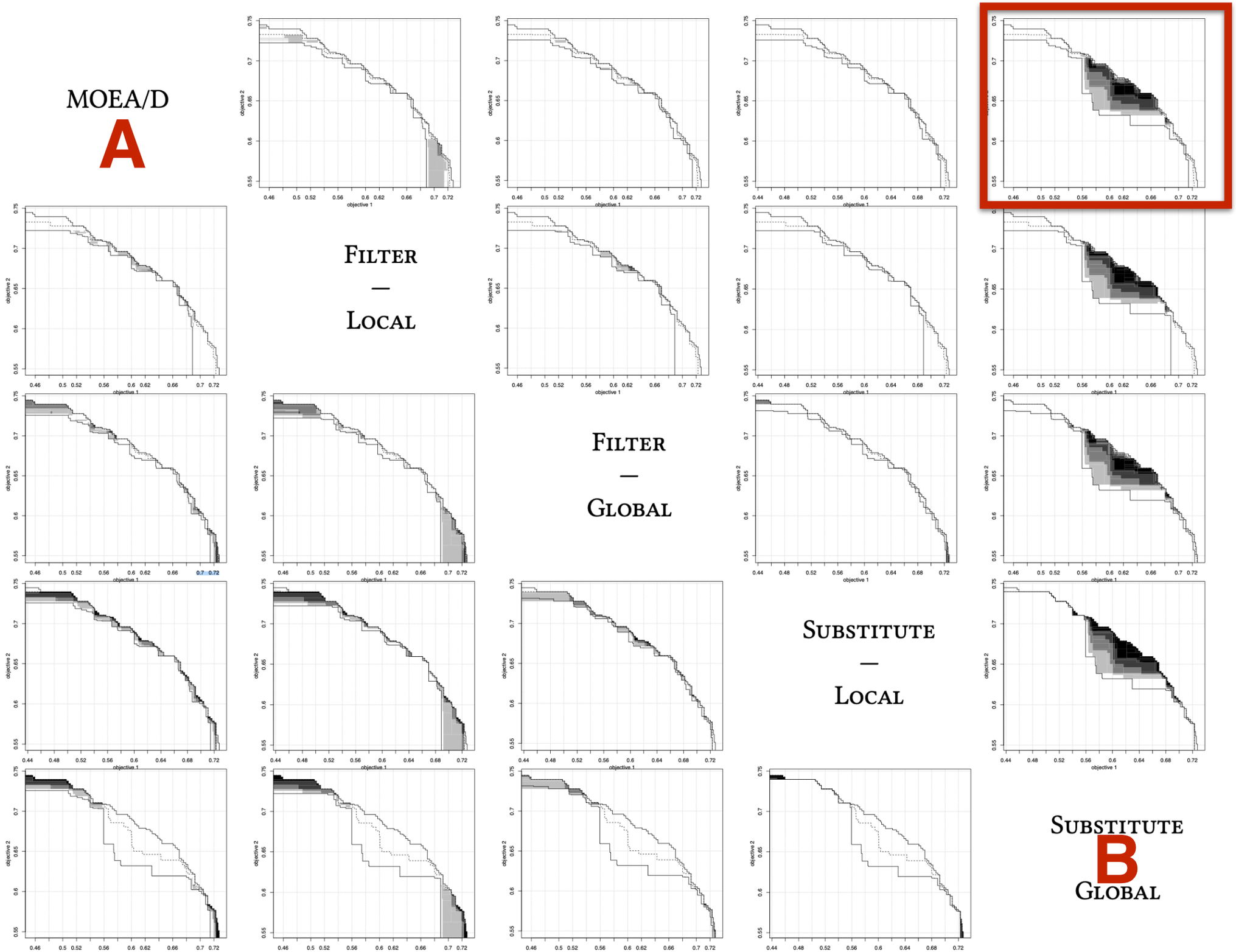
Impact of the selection strategy

Local or Global ?



Impact of the selection strategy

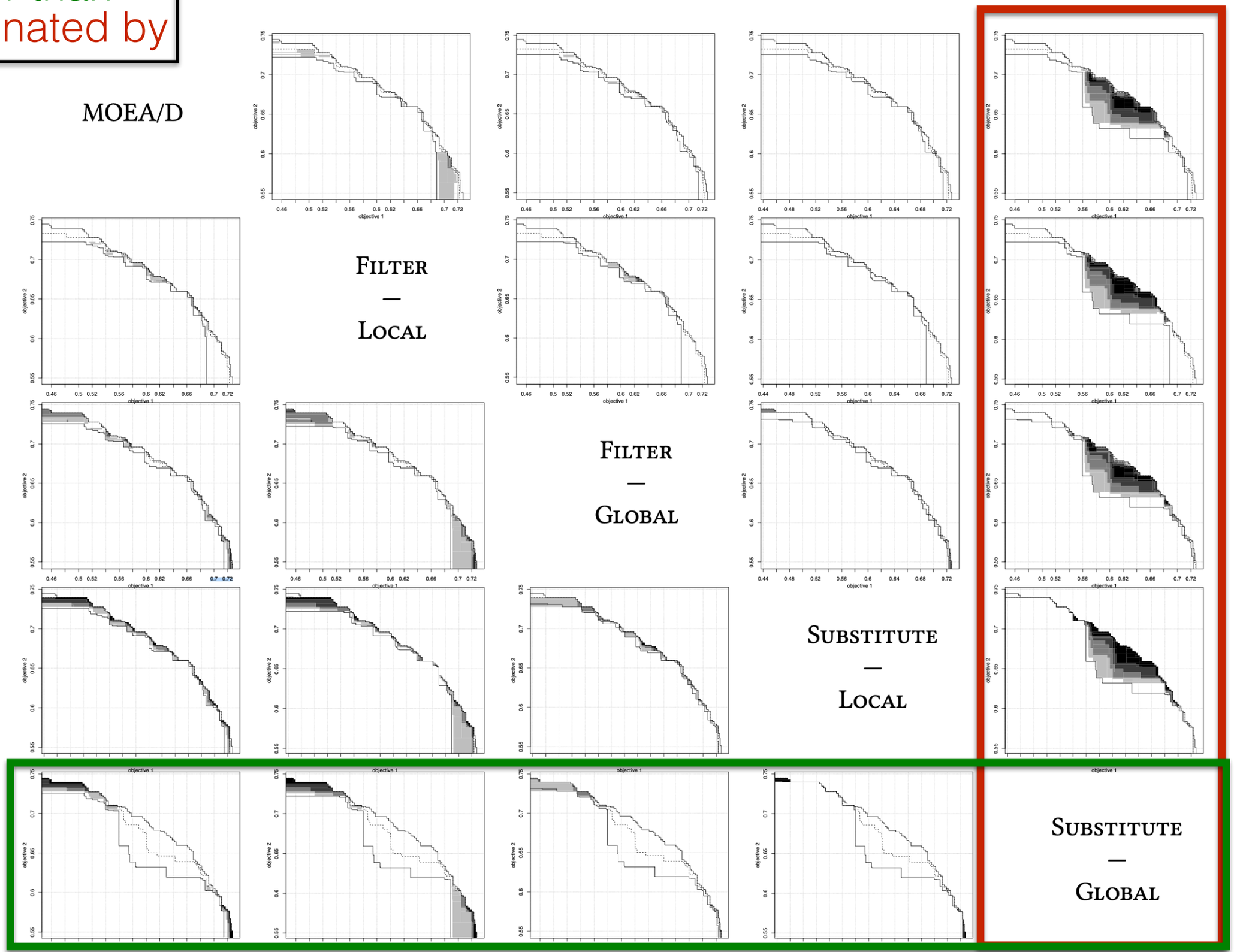
Local or Global ?



Impact of the selection strategy

Local or Global ?

is better than
is dominated by



Impact of the selection strategy

Local or Global ?

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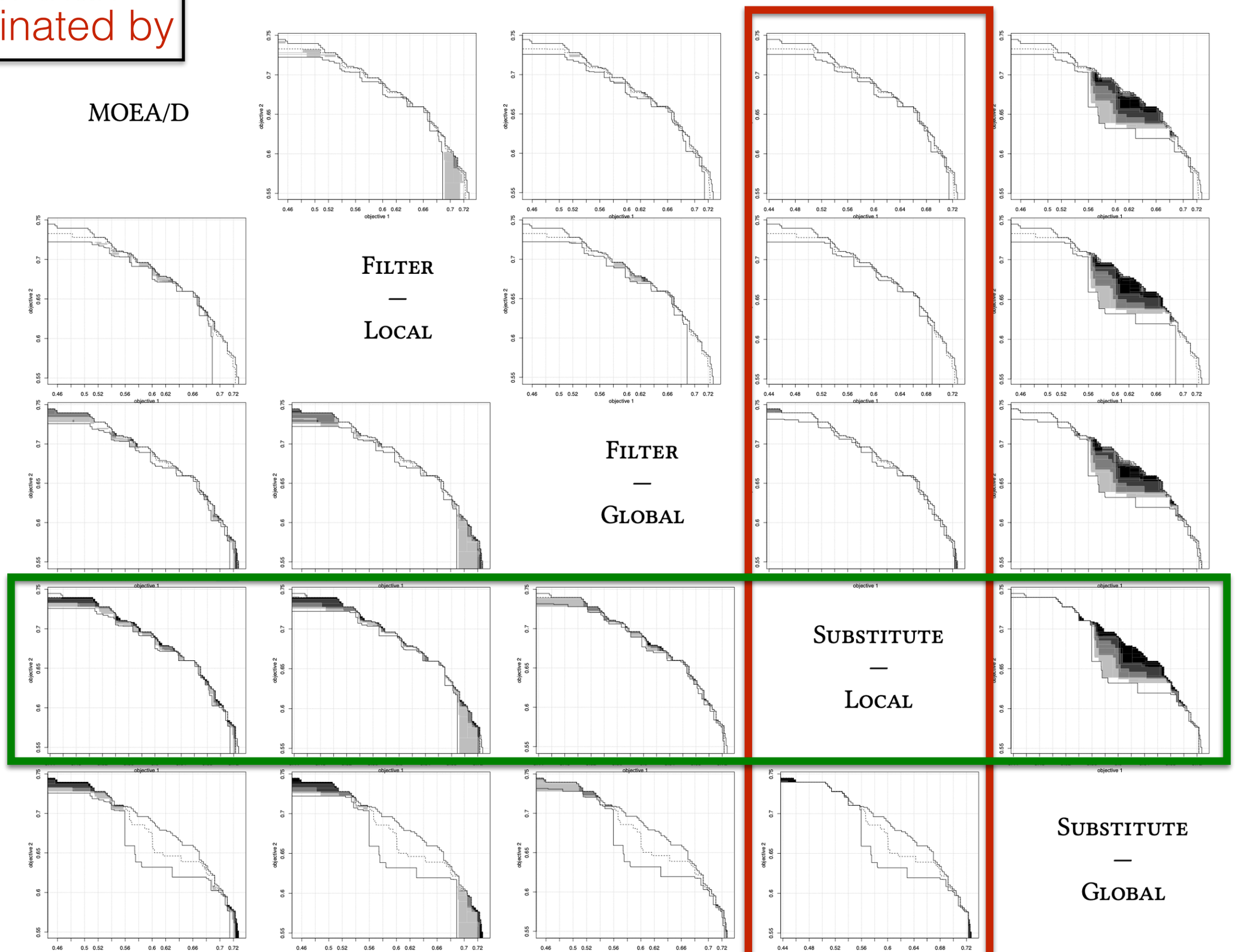
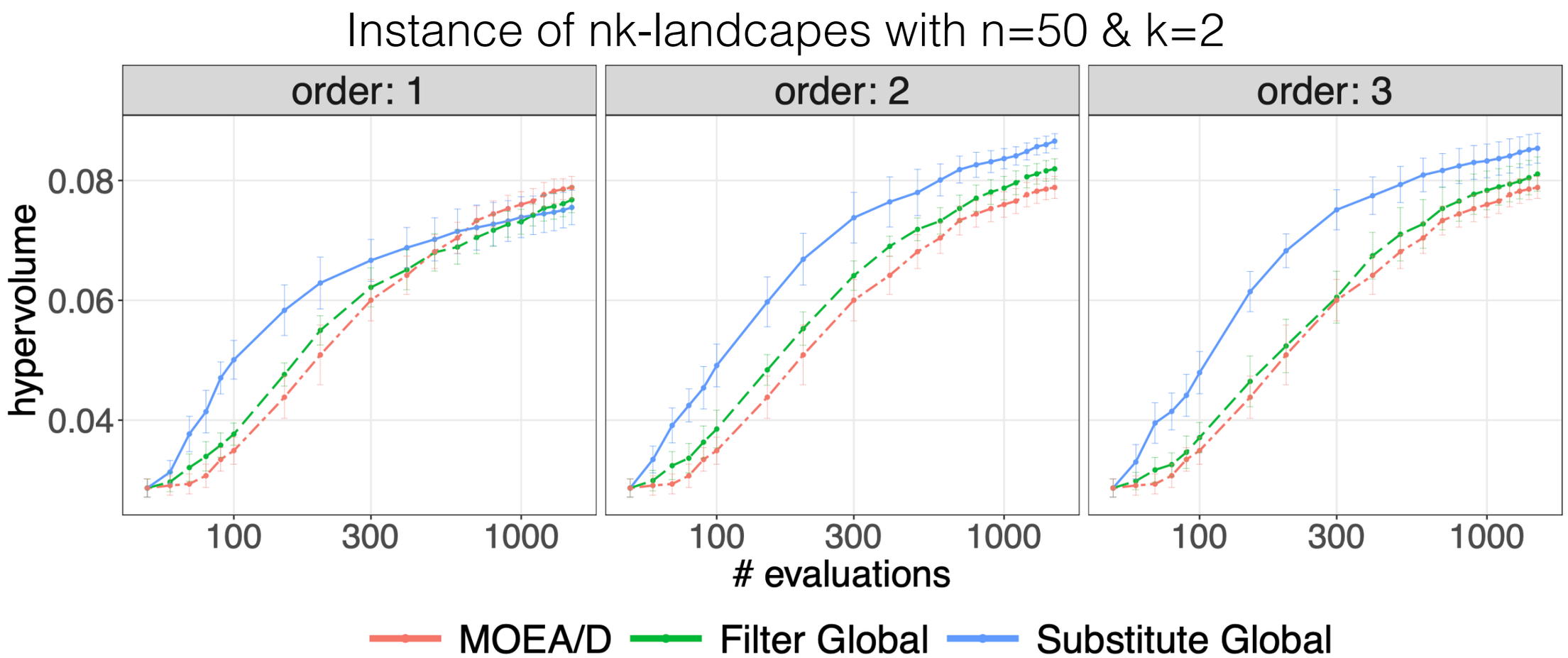


Impact of the Search Engine

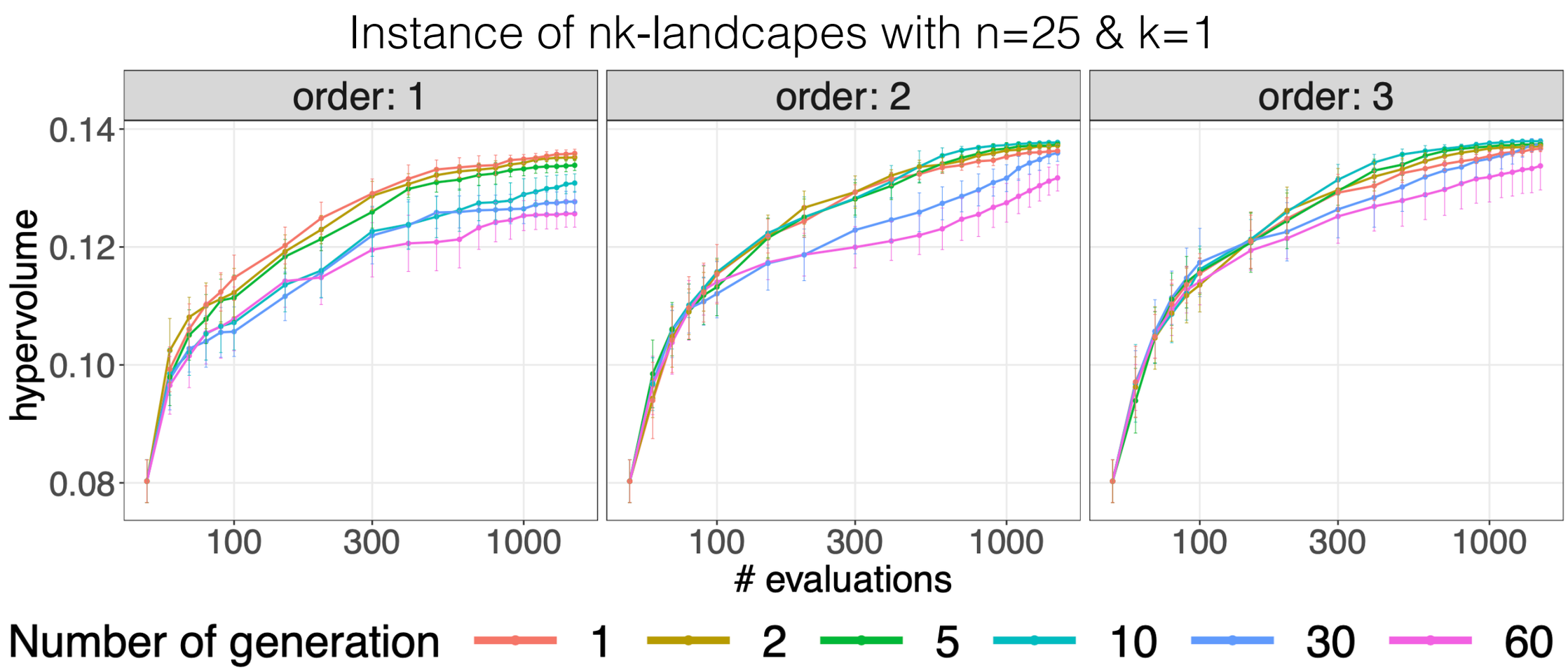
Filtering or Substitution ?



- The substitute search engine seems to be the best (except with a bad Walsh order)
- The main disadvantage : the runtime !

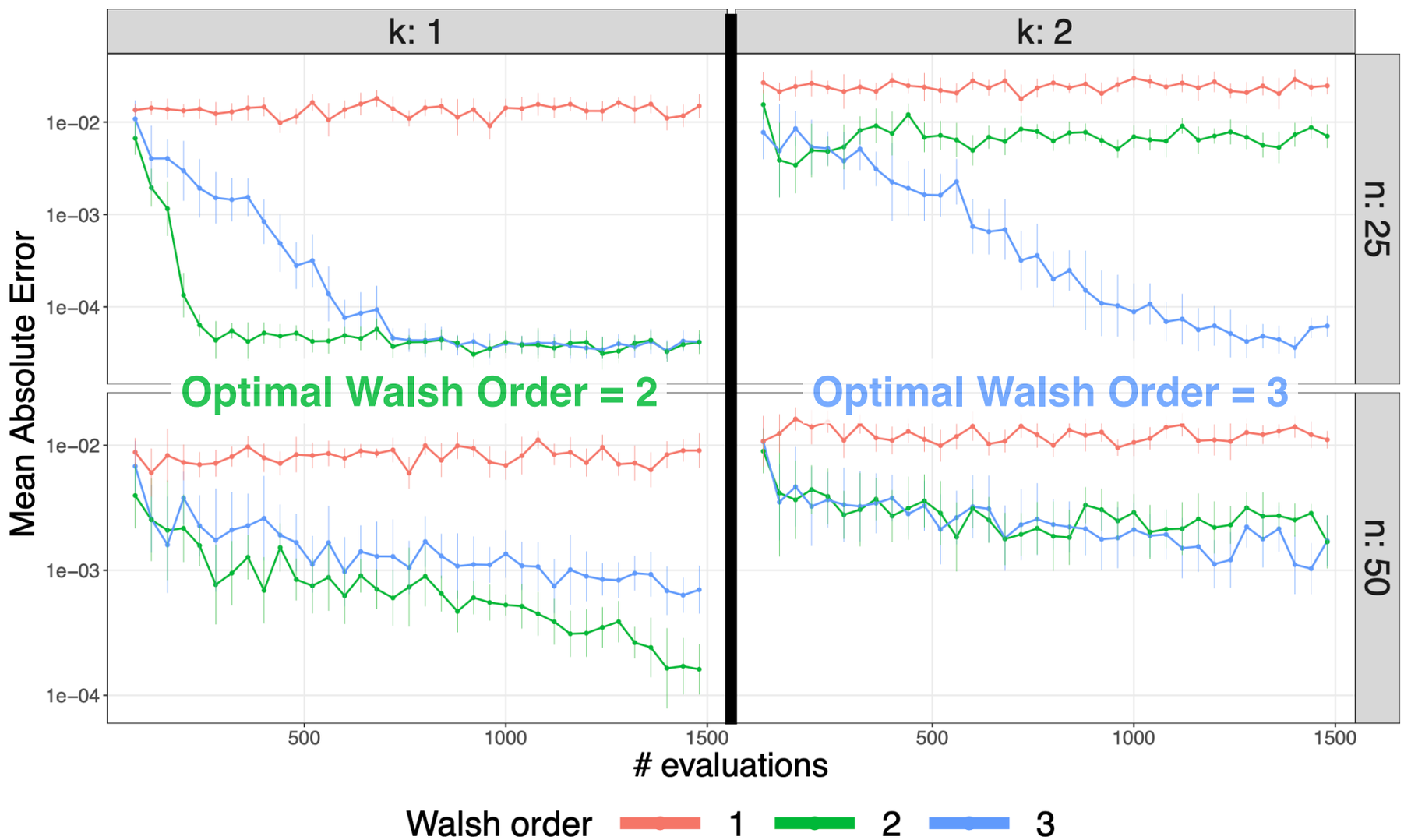
Impact of the Search Engine

Filtering or Substitution ?



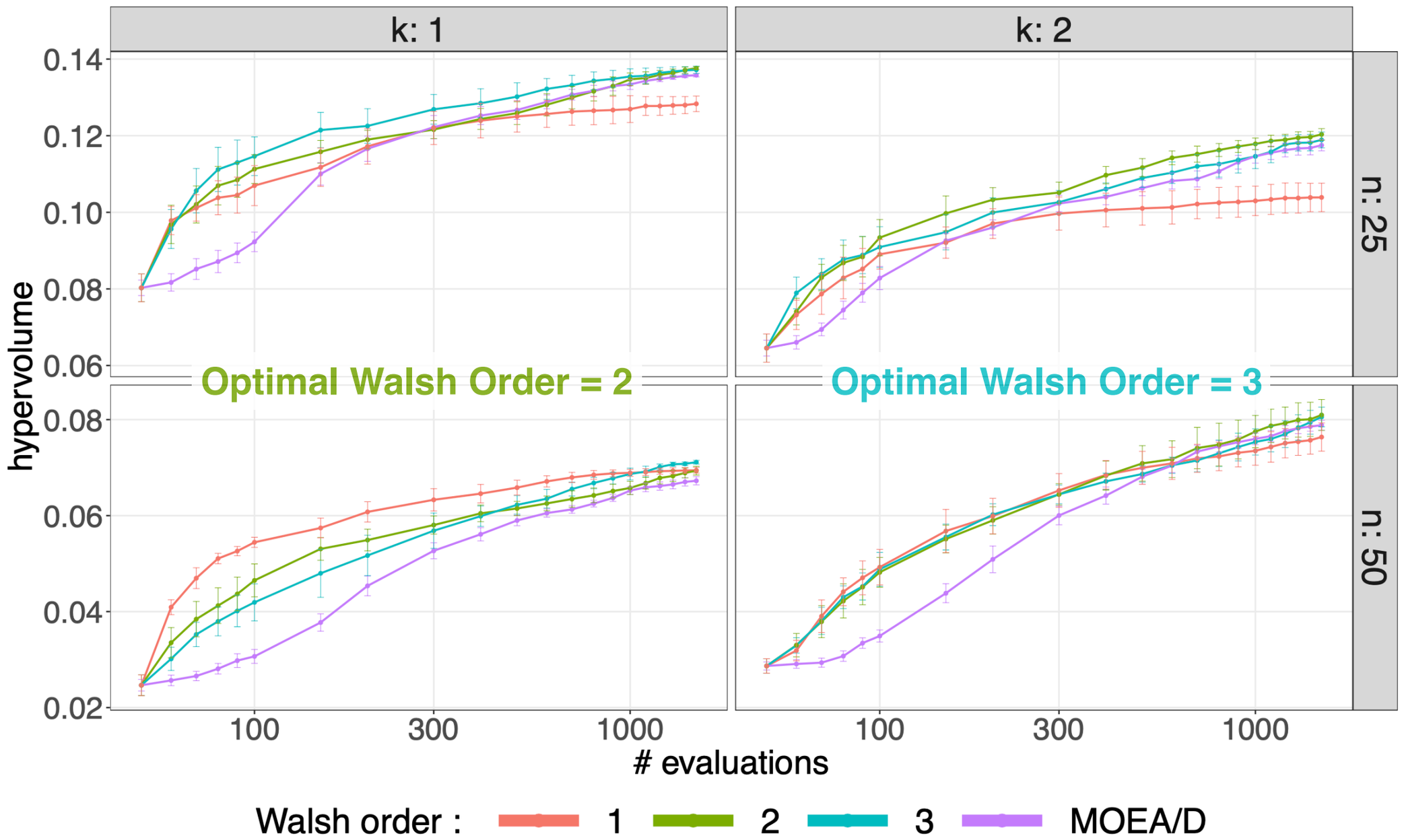
- A low value of g is sufficient
- If the value is to high, the quality is reduced

Impact of the Walsh Order



- The optimal value of the Walsh order d is in theory : $d \geq k + 1$
- Underestimating the order value always decrease the model accuracy
- Overestimating the order value has a tendency to decrease the model accuracy

Impact of the Walsh Order



- These results are not correlated with the accuracy of the problem
- An underestimated order is a viable alternative

Conclusion

- We proposed and analyzed a framework for *discrete surrogate-assisted* multi-objective optimization
- Configuring *decomposition components* and *Walsh surrogates* can impact the behavior of the multi-objective optimization process
- Future research direction :
    - Study the computational budget of decomposition components
    - Study online approaches to adjust components of decomposition and Walsh surrogates

Thank you

Website : https://geoffreypruvost.fr

Email : geoffrey.pruvost@inria.fr

Université de Lille

CRIStAL
Centre de Recherche en Informatique, Signal et Automatique de Lille

cnrs

Inria