Trust-Region Based Multi-Objective Optimization for Low Budget Scenarios

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Outlines

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- Metamodeling for Multi-Objective Optimization
- A Taxonomy for Metamodeling Frameworks for Evolutionary Multi-Objective Optimization
- Metamodeling Framework
- Trust Region based method
- Switching Between Frameworks and Use of Trust Regions
- Results and Comparison
- Conclusions

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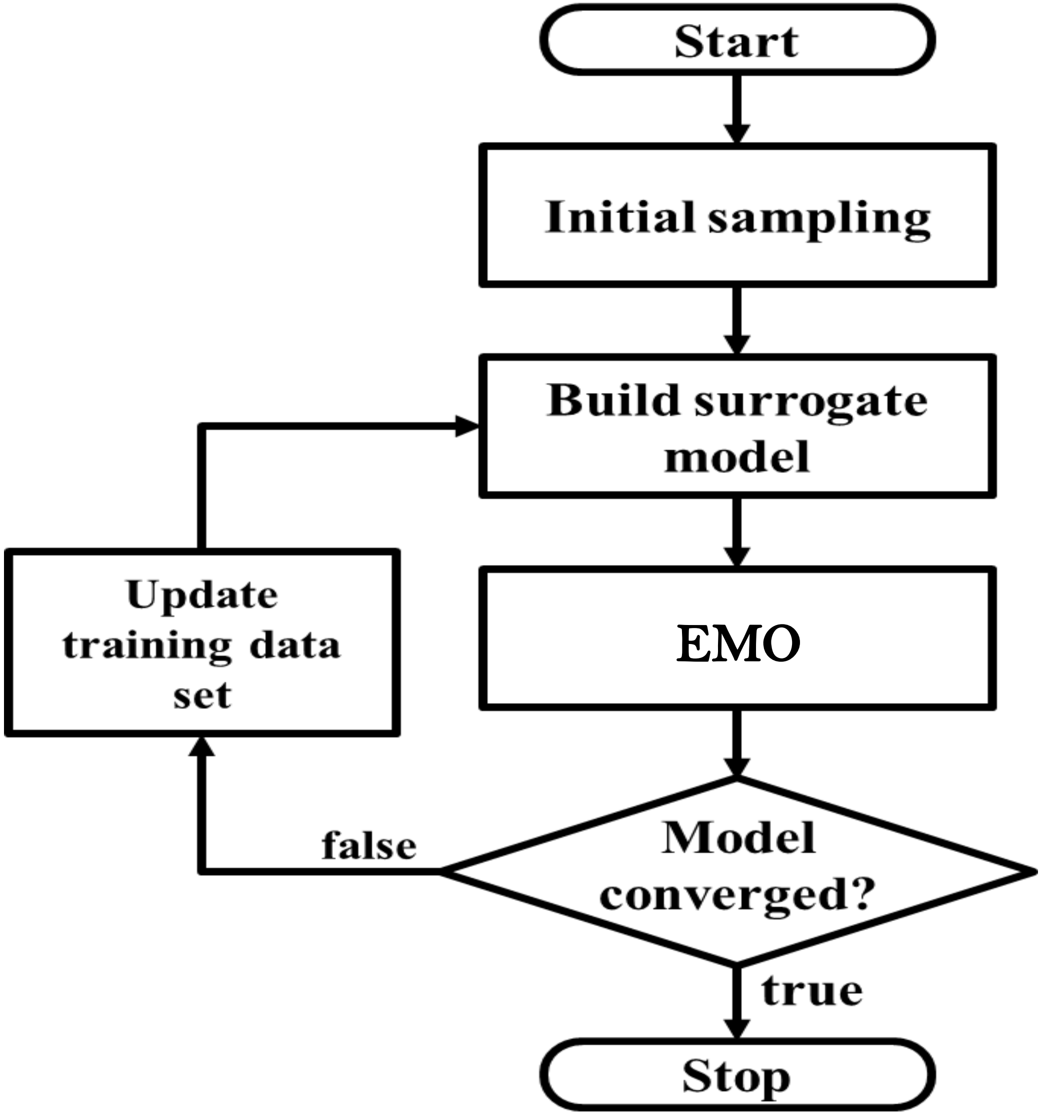
Metamodeling = Surrogate Model = Approximation Model

- Solution evaluations are computationally expensive in practice (Network flow simulation, CFD)
- Single-objective methods may not be straightforward or easy to extend to EMO
- Multiple solutions are targeted
- Metamodels are not accurate
- Multiple objectives and constraints to be meta-modeled
- Constraint handling must be integral part of metamodeling (often ignored)

1. LHS sampling & evaluation (High-Fidelity), sent to **Archive**
2. Build surrogate model(s) for objective(s) and constraint(s)
3. EMO
4. Return **one/multiple** solution(s) & evaluation (High-Fidelity), include in **Archive**
5. Go to step 2



Choices of Metamodel Based Optimization

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1

What functions should be metamodeled?

All Objectives?
All Constraints?
Or their aggregation?

4

Which Optimization Algorithm?

NSGA-III, MOEA/D, RVEA

2

Best Metamodel approach?

RBF, Kriging, NN?

3

How many times? Fixed or Temporal?

When to use what

Taxonomy of Metamodeling Frameworks

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Objectives Separately
M-Metamodels

$(f_1(x), f_2(x), \ldots, f_M(x))$

Aggregated Objective Function
1-Metamodel

ASF(x)

Combine Obj. & Constr., target 1 optimum
1-Metamodel

ASF(x)+CV(x)

Constraints Separately
J-Metamodels

$g_j(\mathbf{x}) \geq 0, \quad \forall j \in \{1, \ldots, J\}$

Constraint Violation Function
1-Metamodel

$\mathrm{CV}(\mathbf{x}) = \sum_{j=1}^{J} \langle \bar{g}_j(\mathbf{x}) \rangle$

Combine Obj. & Constr., target multiple optimum
1-Metamodel

$\mathrm{Min}_h\ \mathrm{ASF}^h(x)+\mathrm{CV}(x)$

Purpose: Construct model search space with different number of metamodels

Better control over search & #metamodels, helps to improve model accuracy

A Taxonomy for Multi-Objective Constrained Problems

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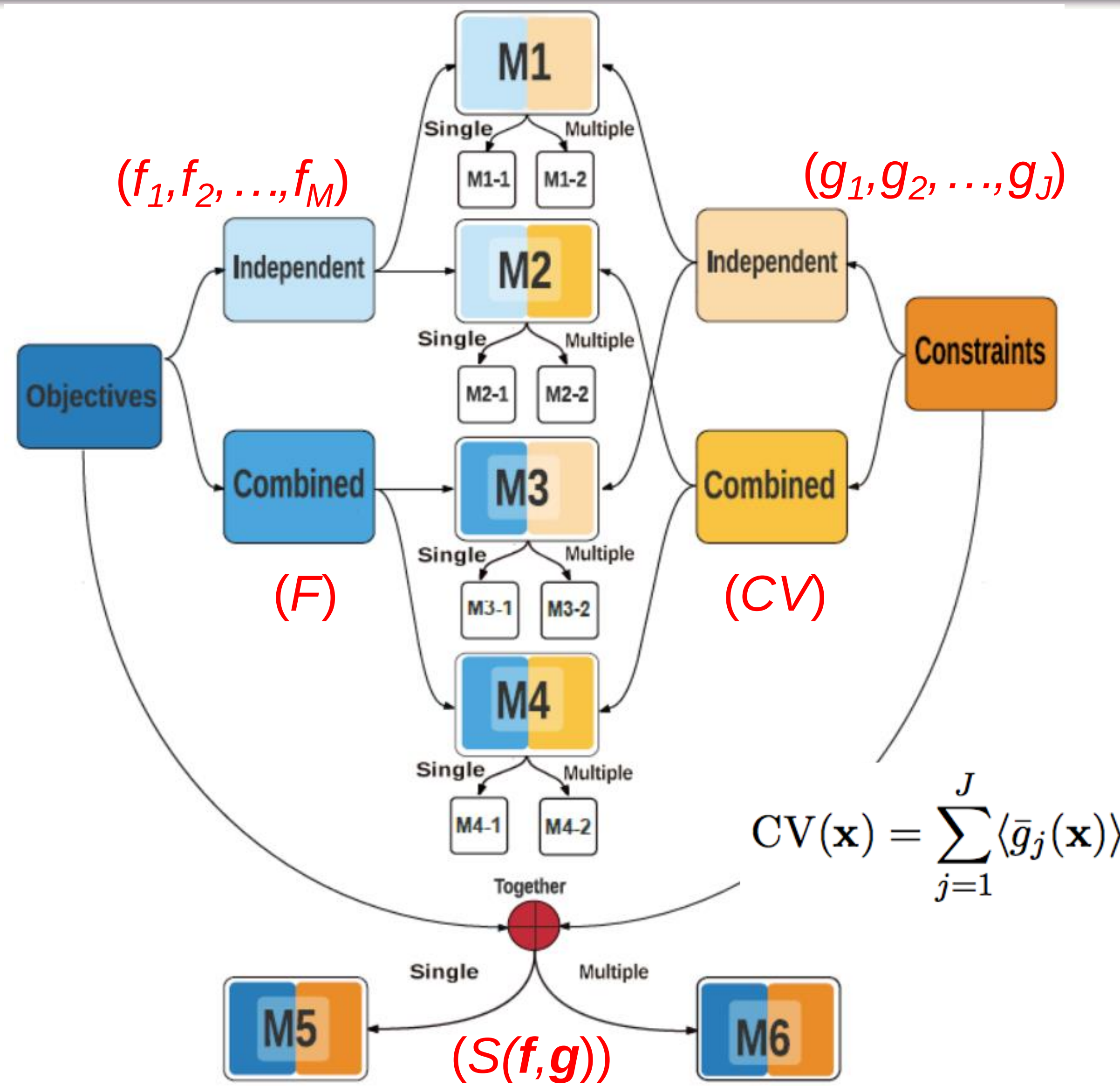
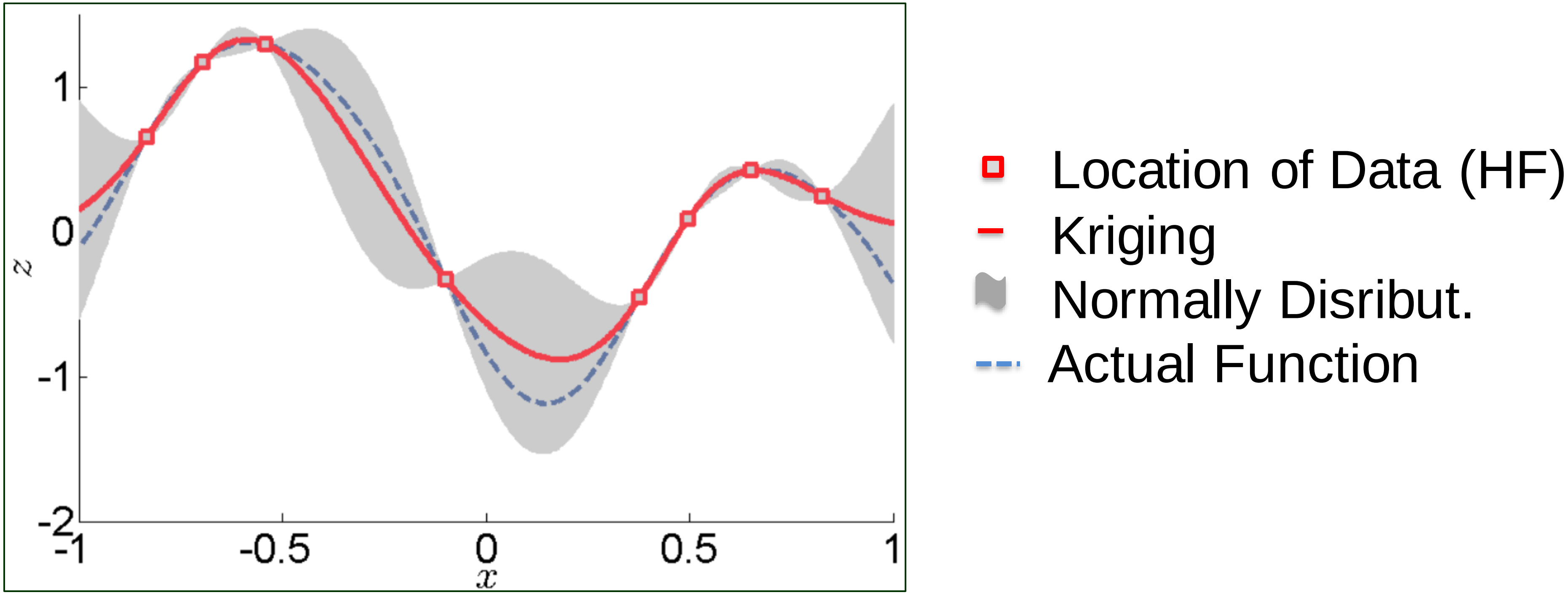


$$\mathrm{CV}(\mathbf{x}) = \sum_{j=1}^{J} \langle \bar{g}_j(\mathbf{x}) \rangle$$

[J] K. Deb, R. Hussein, P. Roy, and G. Toscano "A Taxonomy for Metamodeling Frameworks for Evolutionary Multi-Objective Optimization" , *Accepted IEEE Transactions on Evolutionary Computation,2018.*

Kriging Predictor: $\hat{y}(x) = \hat{\mu} + r(x^*, x)^T R^{-1}(y(x) - \mathbf{1}\hat{\mu})$

Error Estimate: $s^2(x) = \hat{\sigma}^2 [1 - r^T R^{-1} r + \frac{(1 - r^T R^{-1} r)^2}{\mathbf{1}^T R^{-1} 1}]$

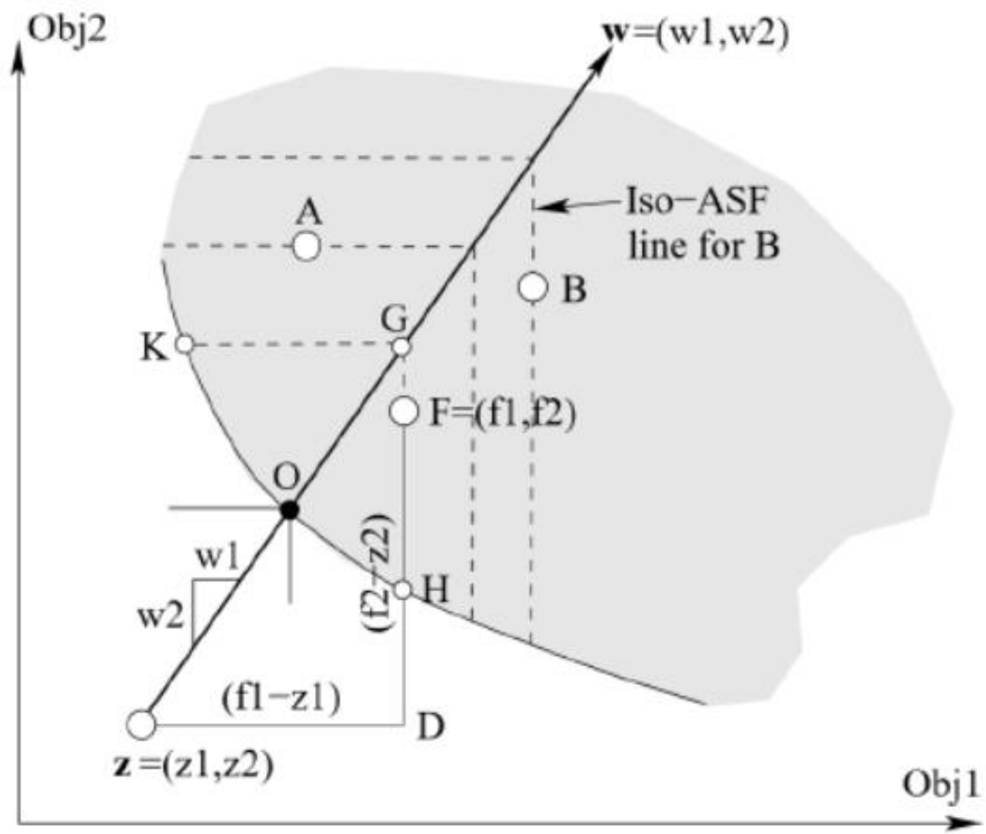


Achievement Scalarization Function (ASF)

- Achievement scalarization method (Wierzbicki, 1980)
- Reference direction ***w*** is changed, reference point ***z*** is fixed to find different PO points
- For a fixed ***z*** and changed ***w*** landscape leads to respective PO point
- It makes monotonic single objective value

$$\text{Minimize}_{(\mathbf{x})} \quad \text{ASF}(\mathbf{x}, \mathbf{z}, \mathbf{w}) = \max_{i=1}^{M} \left(\frac{f_i(\mathbf{x}) - z_i}{w_i} \right),$$

$$\text{Subject to} \quad g_j(\mathbf{x}) \leq 0, \quad j = 1, 2, \ldots, J.$$

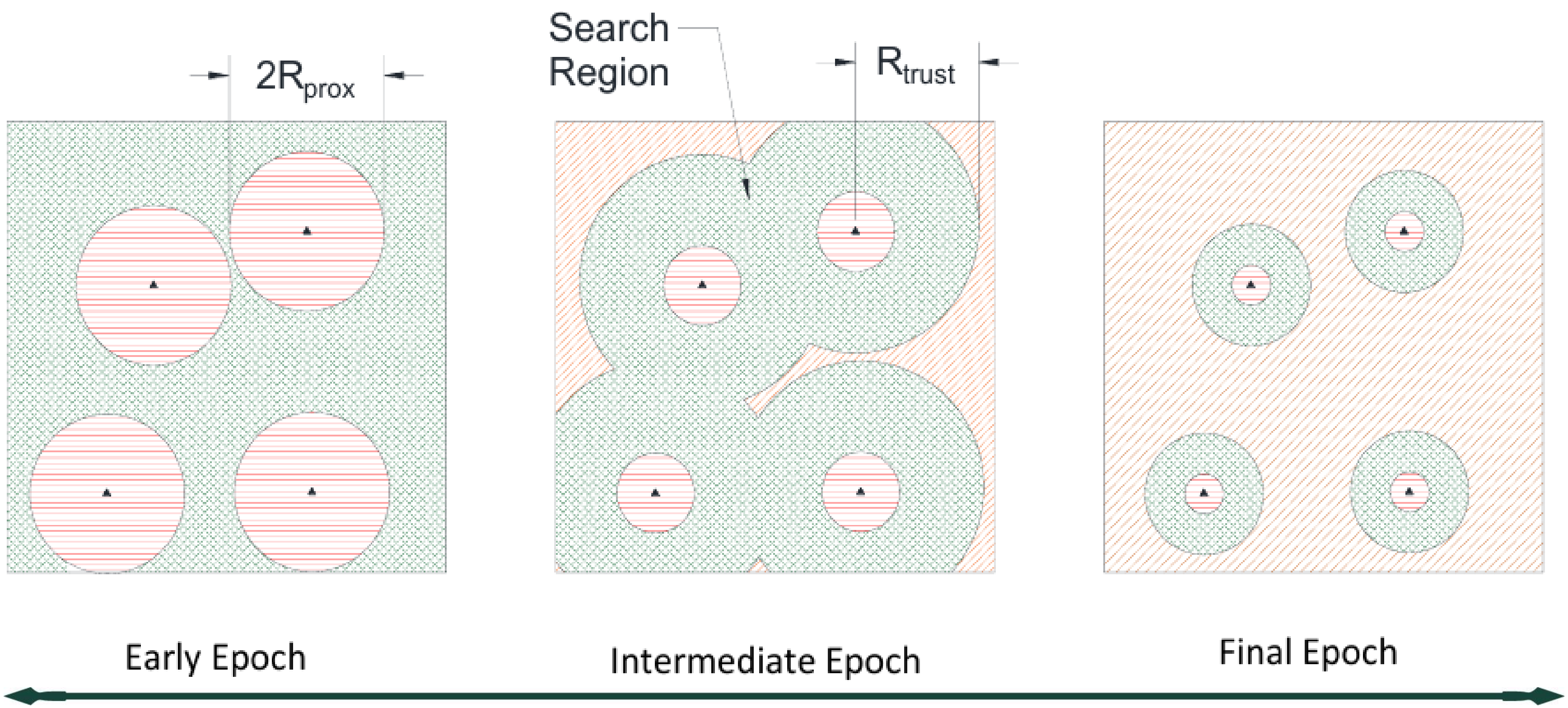


A. P. Wierzbicki, “The use of reference objectives in multiobjective optimization," in Multiple criteria decision making theory and application. Springer, 1980.

Trust Regions

- Maintain a balance between exploration versus exploitation
- Reduce the two radii (R_{trust} and R_{Prox}) after every metamodeling task by constant factors:

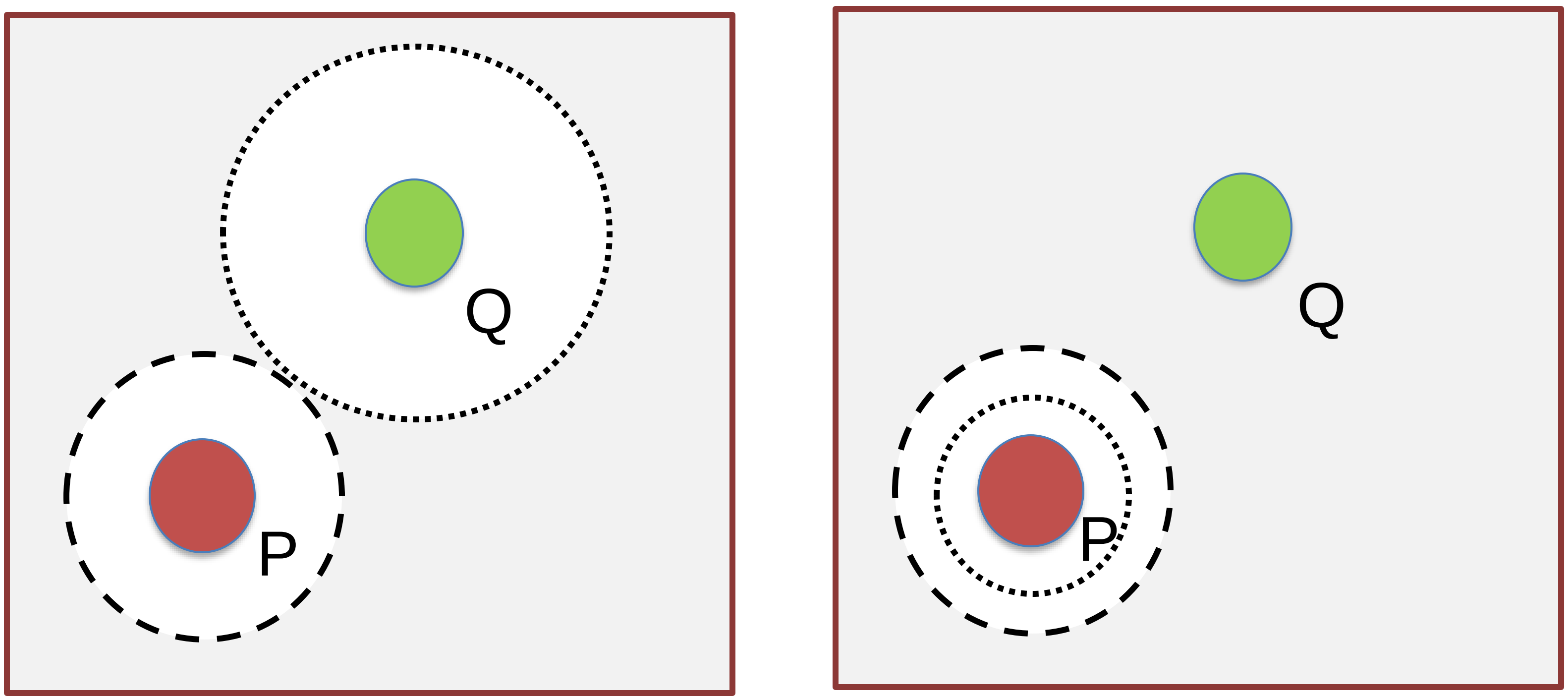
$$R_{trust}^{new} = 0.75 R_{trust}^{old} \qquad R_{prox}^{new} = 0.1 R_{trust}^{new} \qquad R_{prox} \leq R_{search} \leq R_{trust}$$



$$\text{Minimize}_q \quad \hat{f}(q), \quad \text{Subject to} \quad \|q - p\| \leq \delta_k.$$

P: The current iterate (solution).
q: The new predicted point.
δ_k: The search is restricted within a radius.

$$r = \frac{f(p) - f(q)}{f(p) - \hat{f}(q)}.$$

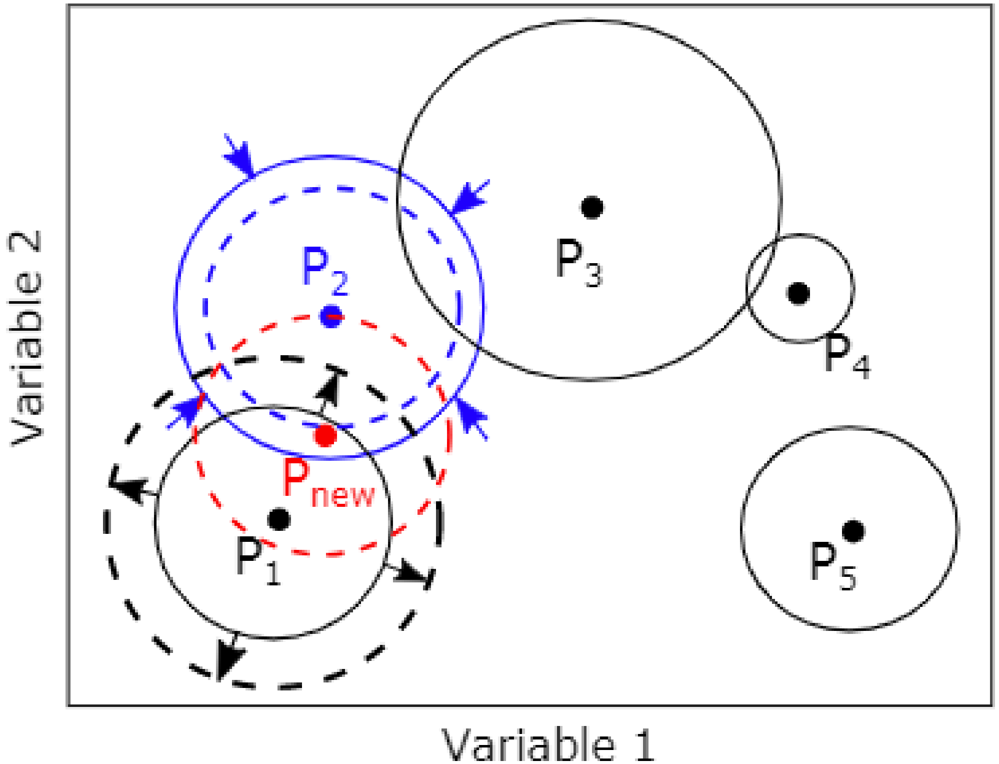


[1] Alexandrov, N.M., Dennis, J.E., Lewis, R.M., Torczon, V.: A trust-region framework for managing the use of approximation models in optimization. Structural optimization (1998)

$$\text{Minimize}_{q \in \Omega} \quad \hat{f}_1(q), \ldots, \hat{f}_M(q)$$

$$\hat{g}_j(x) \geq 0, \quad \forall j \in \{1, \ldots, J\}$$

$$\text{Subject to} \quad \|q - p\| \leq \delta_k^p, \quad \exists p \in A$$



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How to Apply Performance Indicator in Multi-Objective Scenario?

$$r = \frac{f(p) - f(q)}{f(p) - \hat{f}(q)}.$$

The proposed performance criteria based on ASF:

$$PI_{ASF}(q) = \frac{ASF(p) - ASF(q)}{ASF(p) - \widehat{ASF}(q)}.$$

$\widehat{ASF}$: is obtained from predicted objectives.

Performance Indicator for Constraints

A=Archive

Hypervolume based Performance Indicator (PI_{HV}):

$$PI_{HV}(q) = \frac{HV(F(A) \cup F(q)) - HV(F(A))}{HV(F(A) \cup \hat{F}(q)) - HV(F(A))}.$$

Performance Indicator for Constrained Problems:

$$PI_{CV}(q) = \frac{CV(G(p)) - CV(G(q))}{CV(G(p)) - CV(\hat{G}(q))}$$

Overall Trust Region Adaptation

$$r = \begin{cases} PI_{HV}(q) \text{ or } PI_{ASF}(q), & \text{if both } p \text{ and } q \text{ feasible}, \\ r_2 + \epsilon, & \text{if } p \text{ infeasible, } q \text{ feasible}, \\ r_1 - \epsilon, & \text{if } p \text{ feasible, } q \text{ infeasible}, \\ PI_{CV}(q), & \text{otherwise}. \end{cases}$$

$$\delta^p_{k+1} = \begin{cases} c_1 \delta^p_k & \text{if } r < r_1 \\ \min\{c_2 \delta^p_k, \Delta_{max}\} & \text{if } r > r_2 \\ \delta^p_k & \text{otherwise} \end{cases}$$

Proposed Overall Algorithm

Algorithm 1: Trust Region Based Algorithm or TR-NSGA-II

Input : Obj: $[f_1, \ldots, f_m]^T$, Constr: $[g_1, \ldots, g_J]^T$, n (vars), ρ (sample size), E (max. high-fidelity SEs), NSGA-II (multi-obj EA) with pop-size μ, number of generation for model optimization τ, other parameters of NSGA-II Γ, Constraint violation function **CV**, Trust region parameters $\delta_{init}, \Delta_{max}, c_1, c_2, r_1$ and r_2

Output: Solution set P_T

$t, e \leftarrow 0$;
$\mathrm{P}_t, \mathrm{F}_t, \mathrm{G}_t \leftarrow \varnothing$;
$\mathrm{P}_{new} \leftarrow \mathrm{LHS}(\rho, n)$`// Initial solutions`
$\delta^\ell \leftarrow \delta_{init}, \forall \ell \in \{1, \ldots, \rho\}$;
while *True* **do**
 $\mathrm{F}^i_{new} \leftarrow f_i(\mathrm{P}_{new}), \forall i \in \{1, \ldots, M\}$`// eval obj.`
 $\mathrm{G}^j_{new} \leftarrow g_j(\mathrm{P}_{new}), \forall j \in \{1, \ldots, J\}$`// eval constr.`
 if $t > 0$ **then**
  $\widehat{\mathrm{F}}^i_{new} \leftarrow \widehat{f}^i_t(\mathrm{P}_{new}), \forall i \in \{1, \ldots, M\}$`// predicted`
  $\widehat{\mathrm{G}}^j_{new} \leftarrow \widehat{g}^j_t(\mathrm{P}_{new}), \forall j \in \{1, \ldots, J\}$`// predicted`
  $\delta \leftarrow \textsc{Update\_TrustRegion}(\mathrm{F}_t, \widehat{\mathrm{F}}_{new}, \mathrm{G}_t, \widehat{\mathrm{G}}_{new}, \delta)$
 end
 $\mathrm{P}_{t+1}, \mathrm{F}_{t+1}, \mathrm{G}_{t+1} \leftarrow (\mathrm{P}_t \cup \mathrm{P}_{new}), (\mathrm{F}_t \cup \mathrm{F}_{new})$ and $(\mathrm{G}_t \cup \mathrm{G}_{new})$;
 $e \leftarrow e + |\mathrm{P}_{new}|$;
 break if $e \geq E$;
 $\widehat{f}^i_{t+1} \leftarrow \textsc{Metamodel}(\mathrm{F}^i_{t+1}), \forall i \in \{1, \ldots, M\}$`// metamodel obj.`
 $\widehat{g}^j_{t+1} \leftarrow \textsc{Metamodel}(\mathrm{G}^j_{t+1}), \forall j \in \{1, \ldots, J\}$`// metamodel constrt.`
 $\mathrm{P}_{new} \leftarrow \text{NSGA-II}(\widehat{f}_{t+1}, \widehat{g}_{t+1}, \mu, \tau, \Gamma, E - e, \mathbf{CV}, \delta)$; `// Optimize model space`
 $t \leftarrow t + 1$;
end
return $\mathrm{P}_T \leftarrow$ filter the best solutions from P_{t+1}

Parameter Settings

Used Parameters-RGA and NSGA-II

- Population size = 10n
- Crossover probability, p_c = 0.9
- Number of generations = 100
- Mutation probability, p_m = 1/n
- Distribution index for SBX, η_{c} = 2
- Distribution index for Polynomial mutation, η_{m} = 20.
- Two objectives unconstrained: ZDT1, ZDT2, ZDT3, ZDT4 and ZDT6. With 10 variables, **500 FE**, and 21 reference directions.
- Two objectives constraint: BNH, SRN, TNK, OSY, and Welded Beam. With original size variables, **500 FE**, and 21 reference directions.

Performance Metrics

- Inverted Generational Distance (IGD)
- Wilcoxon signed-ranked (p-value)

Results: Two Objective Unconstrained problems

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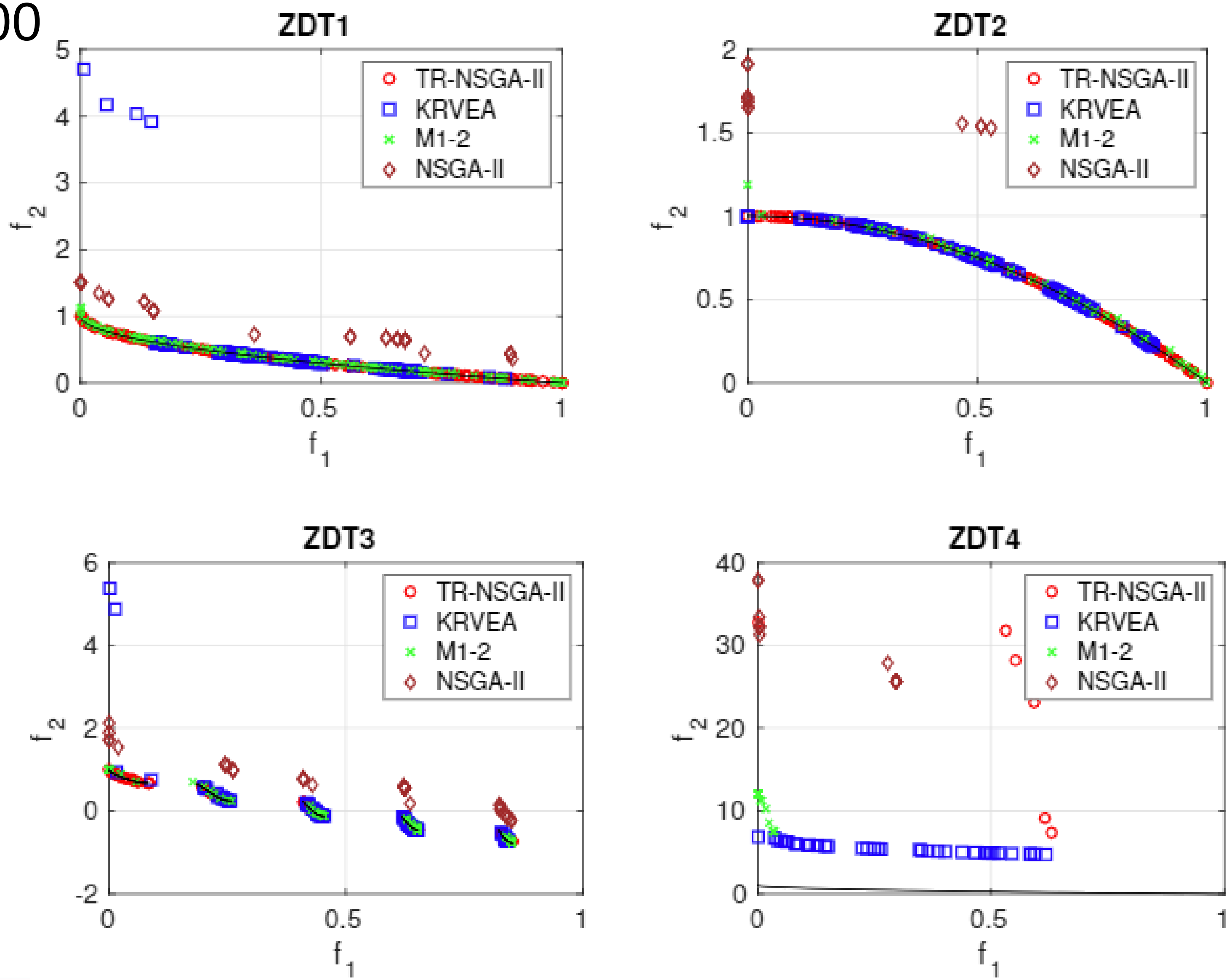
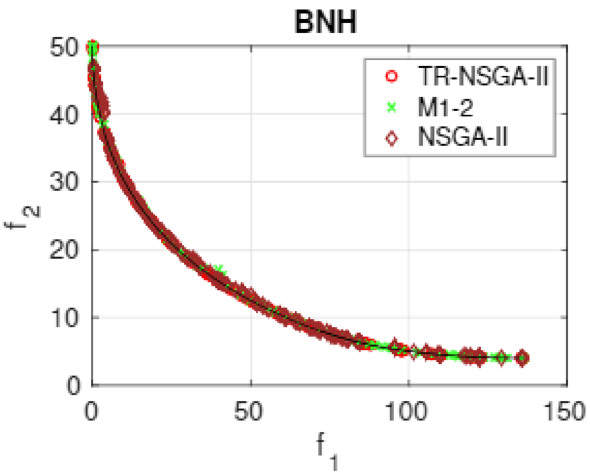
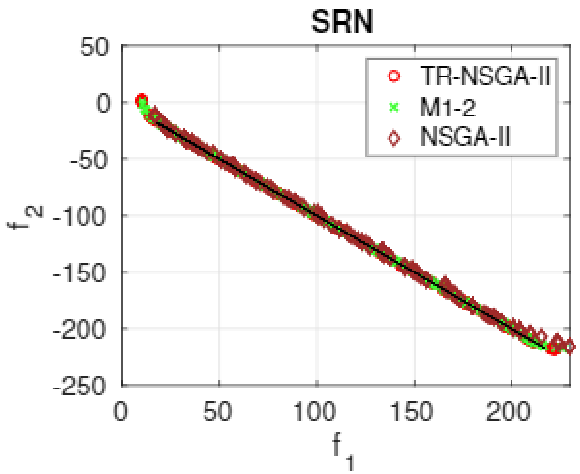
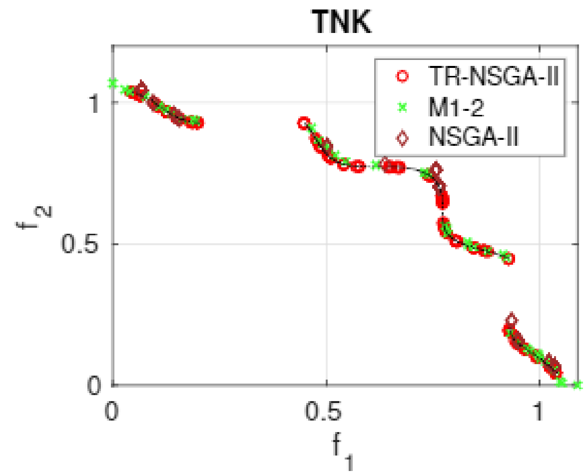
FE=500



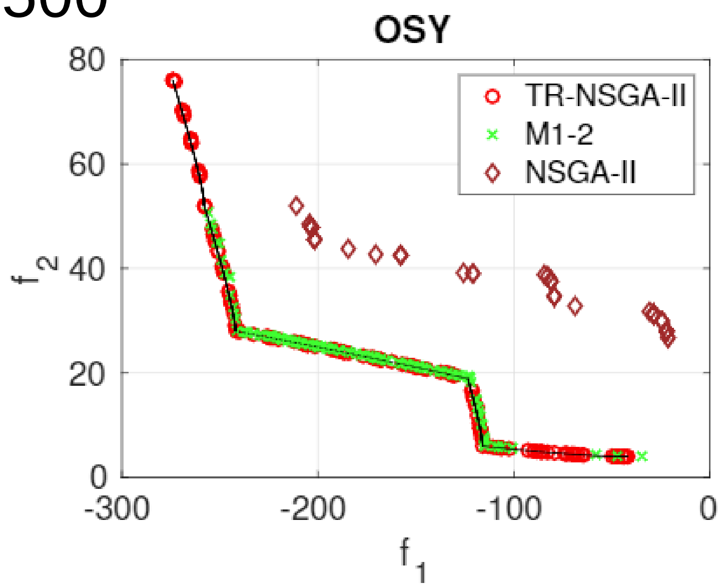
Results: Two Objective Constrained problems

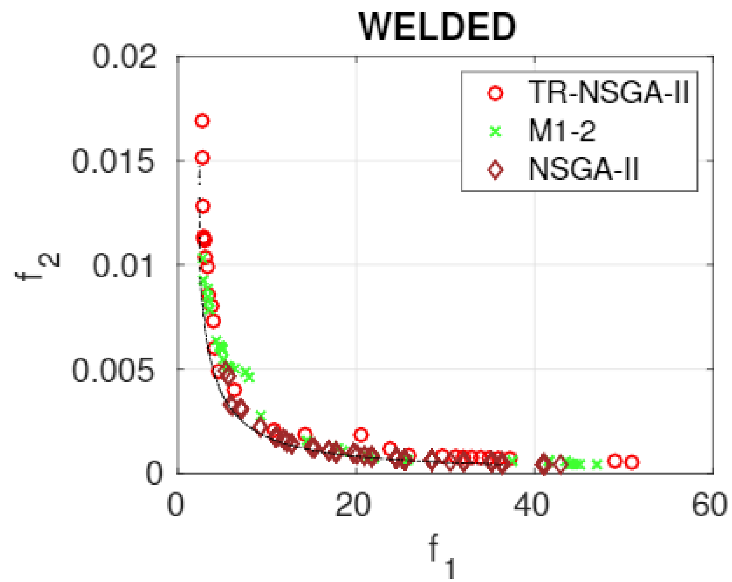






FE=500

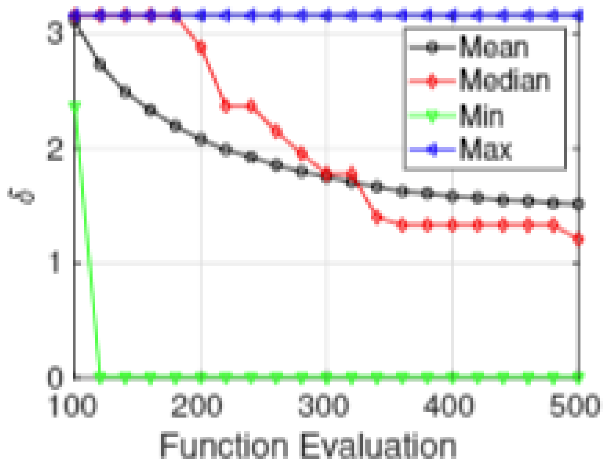




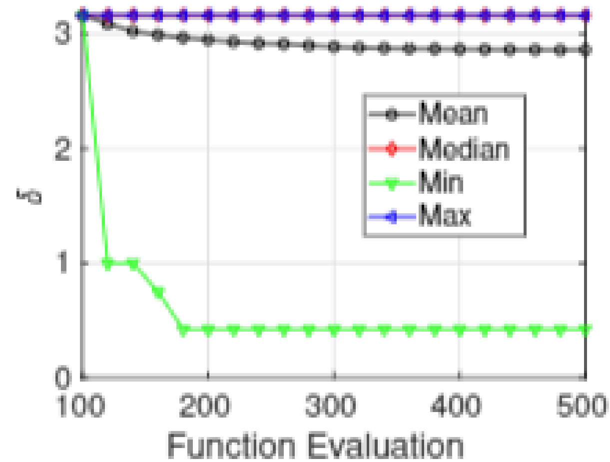
IGD and GD Comparison

Problem/Method	NSGA-II		M1-2		TR-NSGA-II		K-RVEA	
	IGD	GD	IGD	GD	IGD	GD	IGD	GD
ZDT1	0.27131	0.34582	0.01161	0.01091	**0.00121**	**0.00122**	0.07964	0.03715
	p=1.852e-05	p=1.852e-05	p=7.7801e-04	p=7.4613e-04	-	-	p=1.852e-05	p=1.852e-05
ZDT2	0.98265	0.61637	0.00975	0.00755	**0.00057**	**0.00081**	0.03395	**0.00080**
	p=1.852e-05	p=1.852e-05	p=1.852e-05	p=1.852e-05	-	p=0.2851	p=1.852e-05	-
ZDT3	0.32080	0.38940	0.01251	0.00761	**0.00870**	**0.00230**	0.02481	0.00650
	p=1.852e-05	p=1.852e-05	p=1.852e-05	p=1.852e-05	-	-	p=1.852e-05	p=1.802e-04
ZDT4	25.24040	34.43350	**7.11881**	**10.10851**	**6.97620**	**12.92170**	**4.33221**	**4.50901**
	p=1.852e-05	p=1.852e-05	p=0.7928	p=0.1007	p=0.8955	p=0.2934	-	-
ZDT6	5.00571	4.80922	1.55861	2.27535	**0.31070**	2.84941	0.65462	**1.50551**
	p=1.852e-05	p=1.852e-05	p=1.852e-05	p=0.001	-	p=0.0151	p=1.852e-05	-
BNH	0.78981	0.19842	0.45272	0.13696	**0.09651**	**0.09092**	-	-
	p=1.852e-05	p=1.852e-05	p=1.852e-05	p=1.852e-05	-	-		
SRN	1.66162	2.11235	**0.67285**	**0.75337**	1.44045	1.74951	-	-
	p=1.852e-05	p=1.852e-05	-	-	p=1.852e-05	p=1.852e-05		
TNK	0.04182	0.01341	0.01543	0.01008	**0.00141**	**0.00201**	-	-
	p=1.852e-05	p=1.852e-05	p=1.852e-05	p=1.852e-05	-	-		
OSY	35.80211	27.43991	4.78063	0.59202	**0.16731**	**0.25063**	-	-
	p=1.852e-05	p=1.852e-05	p=1.852e-05	p=1.852e-05	-	-		
Welded Beam	1.10272	**0.21092**	0.92692	1.68806	**0.07681**	1.72811	-	-
	p=1.852e-05	-	p=1.8267e-04	p= 0.0042	-	p=0.0012		
C2DTLZ2	0.13733	0.04792	**0.03355**	**0.02373**	0.06411	0.02991	-	-
	p=1.852e-05	p=1.852e-05	-	-	p=1.8267e-04	p=1.8267e-04		

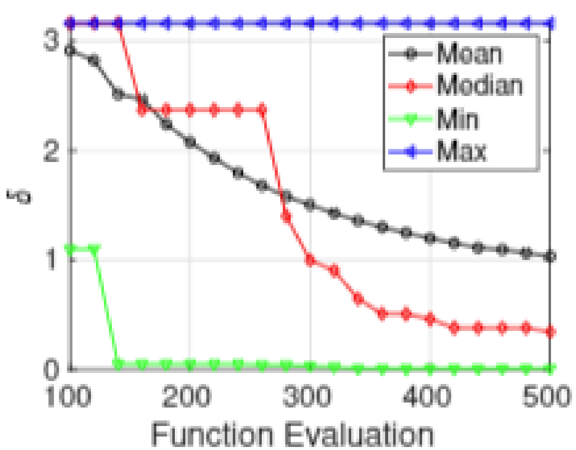
Trust Region Adaptation



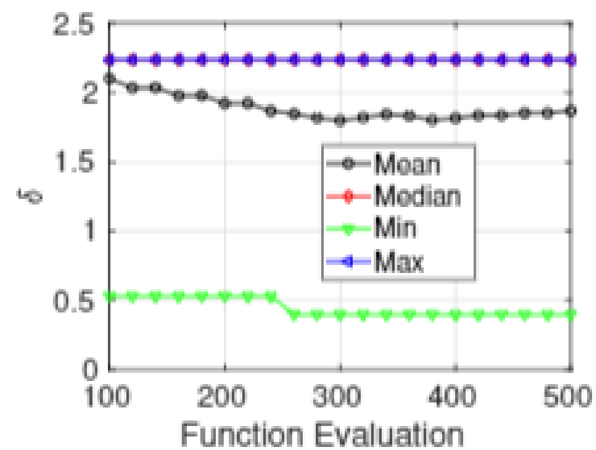
ZDT1



ZDT3



ZDT4

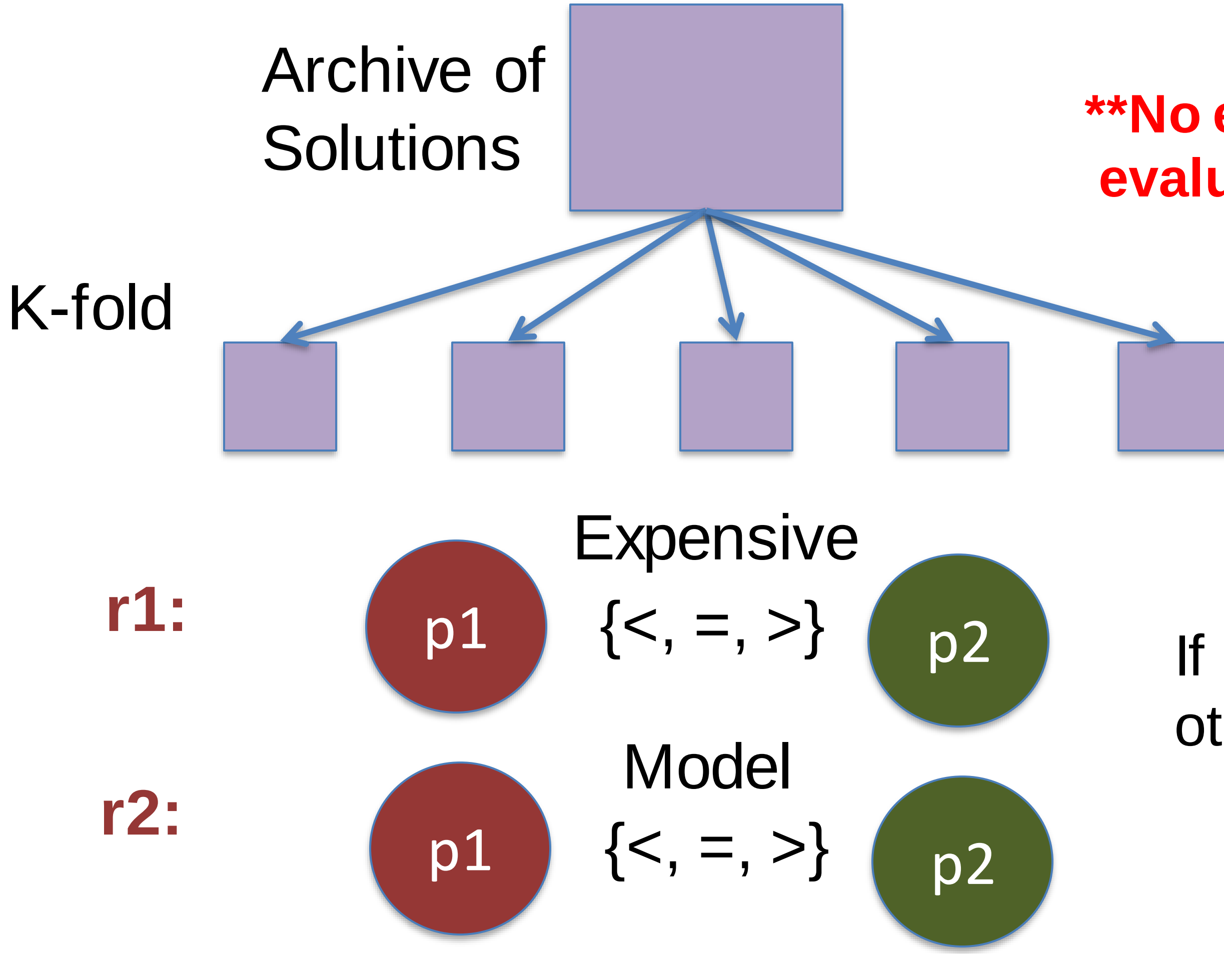


ZDT6

Switching Between Frameworks

- It is more efficient to use different metamodeling frameworks at different stages of the optimization process.
- Adaptive Switching Mechanisms: Ensemble-based method involving different metamodeling frameworks.
- Implemented the trust regions concept for getting more robust solutions and reduce the uncertainty as well.

Adaptive Switching Method

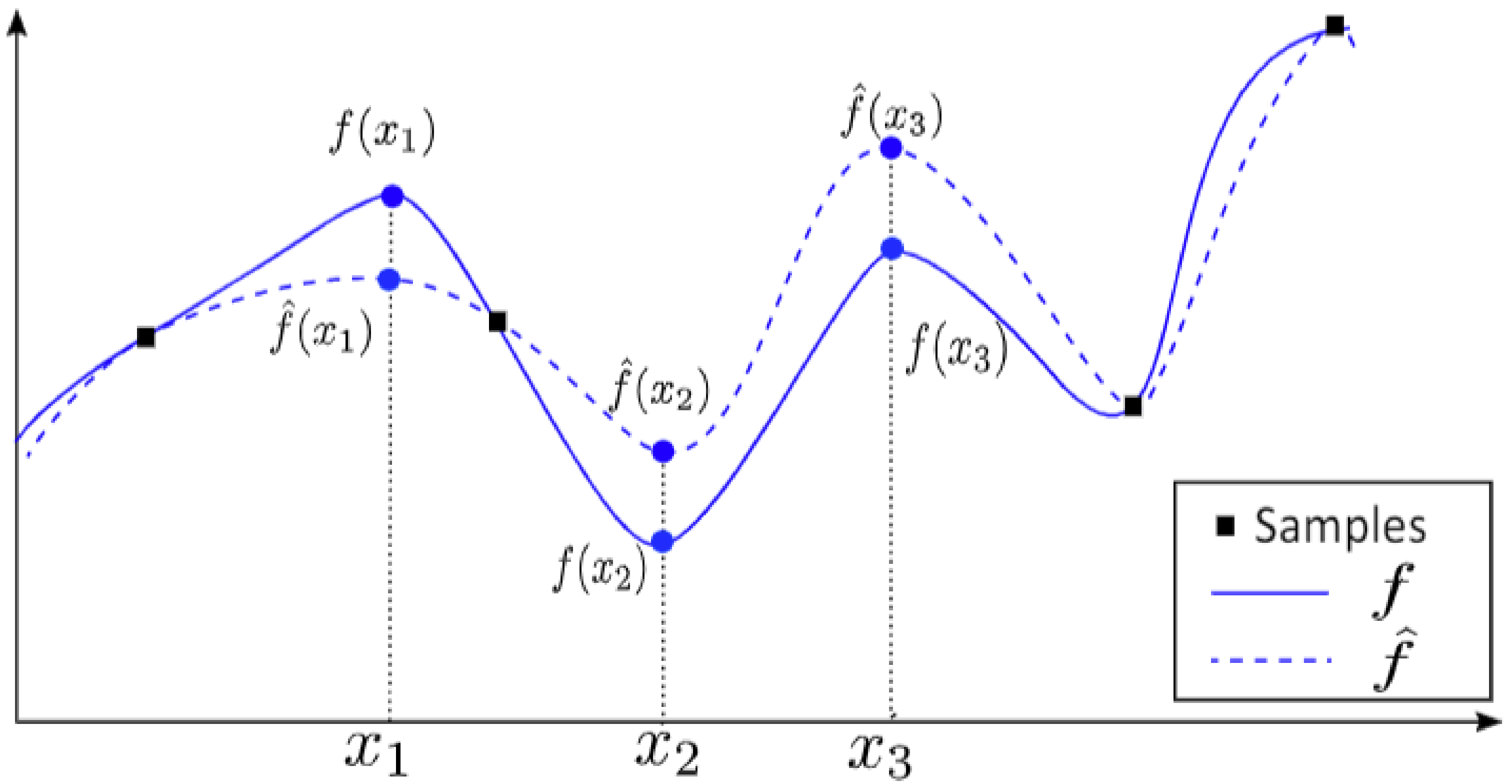


****No exact solution evaluation needed**

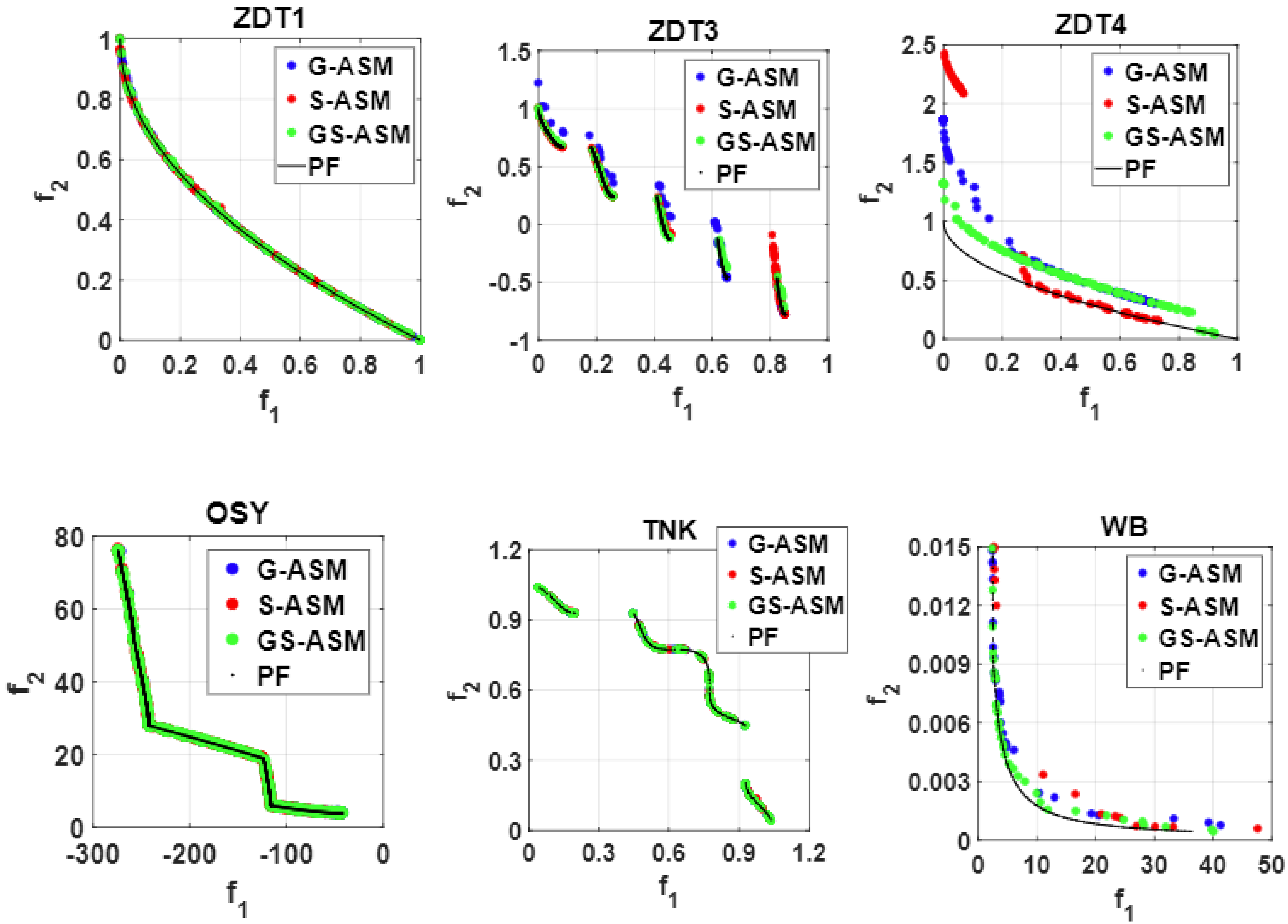
If **r1** =**r2,** no error, otherwise error

$$\text{Selection Error Probability (SEP)} = \frac{Error\ Count}{\binom{|Test\ Data|}{2}}$$

Selection Error Probability: Pairwise comparison between high-fidelity and prediction values (metamodeling)



Results of Adaptive Switching Method



Median IGD run for ZDT3 test problem

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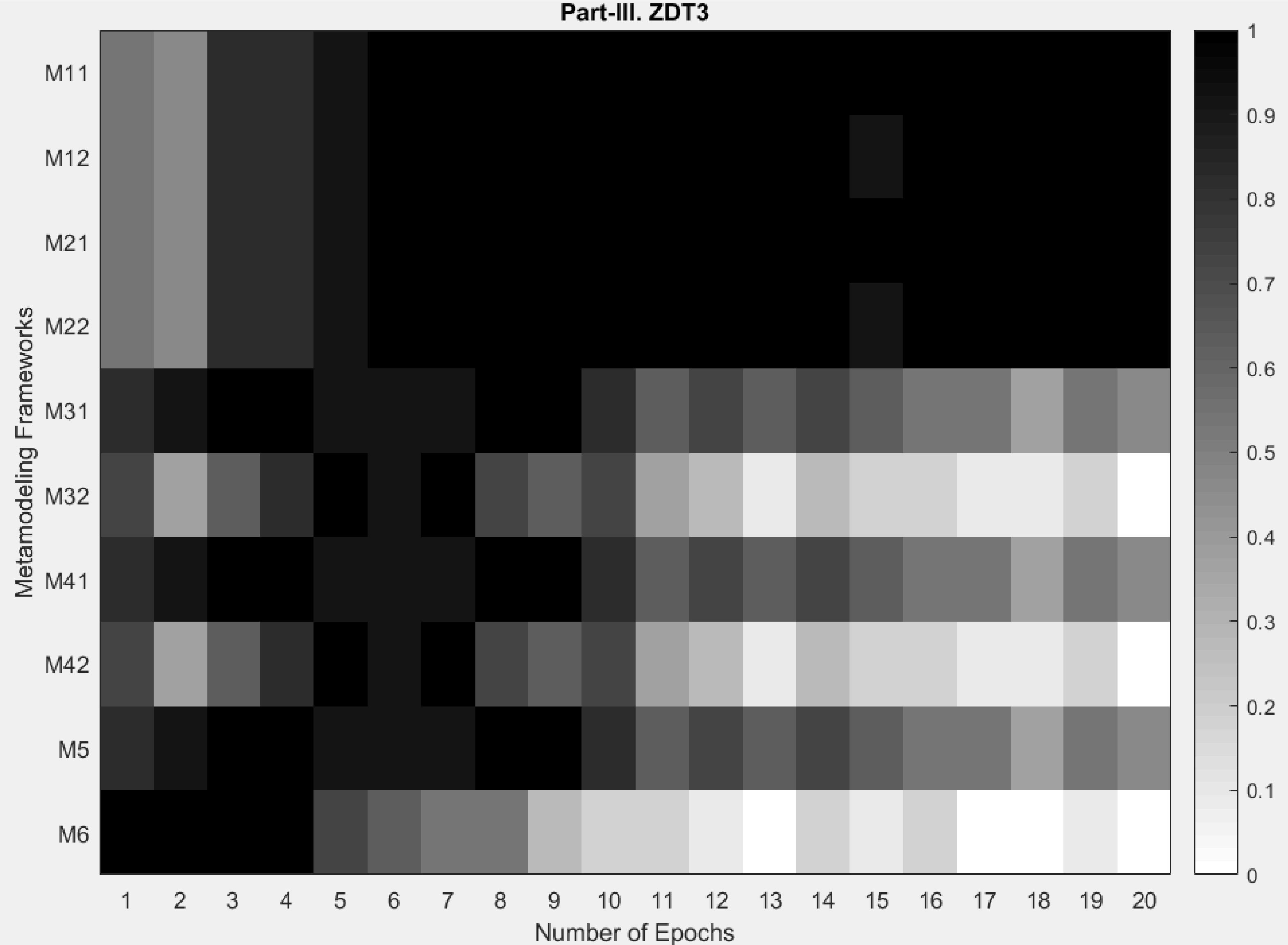
	ZDT3-500 FEs ,IGD: 0.0039823, GD: 0.0015807																			
Frameworks	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
M1-1																				
M1-2																				
M2-1																				
M3-1																				
M4-1																				
M5																				

	ZDT3-500 FEs ,IGD: 0.0039823, GD: 0.0015807																			
Frameworks	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
M1-2																				
M2-2																				
M3-2																				
M4-2																				
M6																				

	ZDT3-500 FEs ,																			
Frameworks	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
M1-1																				
M1-2																				
M2-1																				
M2-2																				
M3-1																				
M3-2																				
M4-1																				
M4-2																				
M5																				
M6																				

Mean run for ZDT3 test problems: Part-III



Results of IGD for Adaptive Switching Method

Problem		MOEA/D-EGO	K-RVEA	CSEA	GS-ASM
ZDT1		0.05611	0.07964	0.95330	**0.00130**
		p=8.1e-5	p=8.1e-5	p=8.1e-5	p=0.0910
ZDT2		0.04922	0.03395	1.01060	**0.00055**
		p=8.1e-5	p=8.1e-5	p=8.1e-5	-
ZDT3		0.30380	0.02481	0.94840	**0.00391**
		p=8.1e-5	p=8.1e-5	p=8.1e-5	-
ZDT4		73.25920	4.33221	12.71600	**0.39992**
		p=8.1e-5	p=8.1e-5	p=8.1e-5	-
ZDT6		0.51472	0.65462	5.42620	**0.24440**
		p=8.1e-5	p=8.1e-5	p=8.1e-5	p= 0.0612
DTLZ2		0.33170	0.0548	0.11420	**0.03701**
		p=8.1e-5	p=8.1e-5	p=8.1e-5	p=0.157
DTLZ4		0.64533	**0.0449**	0.08110	0.07934
		p=8.1e-5	-	p=0.0022	p=0.0380
DTLZ5		0.26203	0.0164	0.03081	**0.01252**
		p=8.1e-5	p=8.1e-5	p=8.1e-5	p=0.211
DTLZ7		5.33220	**0.0531**	0.70520	**0.06529**
		p=8.1e-5	-	p=8.1e-5	p=0.1930

Median IGD on unconstrained problems using GS-ASM and MOEA/D-EGO, K-RVEA, and CSEA algorithms.

Conclusions

- Trust regions are used as a constraint in the variable space during optimization to deal with uncertainties of metamodels.
- Proposed two performance indicators based on ASF & Hypervolume to adapt trust regions.
- A constraint handling scheme is presented to handle the trust region adaptation for constrained problems
- A multiple trust regions implemented with multiple trade-off solutions.
- Our results on several test multiobjective optimization problems have shown that we can achieve better convergence using the proposed method than that without a trust region.

Reference

- "A Taxonomy for Metamodeling Frameworks for Evolutionary Multiobjective Optimization"- K. Deb, R. Hussein, PC Roy, G. Toscano-Pulido
- "Adaptive Switching Strategy for Metamodeling Based Multi-objective Optimization: Part I, Generative Frameworks" R. Hussein, K. Deb and PC Roy
- "Adaptive Switching Strategy for Metamodeling Based Multi-objective Optimization: Part II, Simultaneous and Combined Frameworks"- PC Roy, R. Hussein, K. Deb
- Github Repo: https://github.com/proteekroy

Questions and Comments?