Tutorial

Evolutionary Multi- and Many-Objective Optimization: Methodologies, Applications and Demonstration

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Outline of the Tutorial

- Multi-objective Optimization (MOO) Basics
- Evol. Multi-criterion Optimization (EMO): Past
- EMO: Present and Future
  - Too many to cover, discuss main current topics
  - Many-objective and massive-objective optimization, Objective reduction, *Innovization*, Distributed computing, Visualization and decision-making, Problems with Uncertainty, Metamodel based EMO, Dynamic EMO, Bilevel EMO, Theoretical convergence measure, knee finding, Test problem construction, Extreme solutions
- Demonstration of **pymoo**: public domain code
  - https://pymoo.org/

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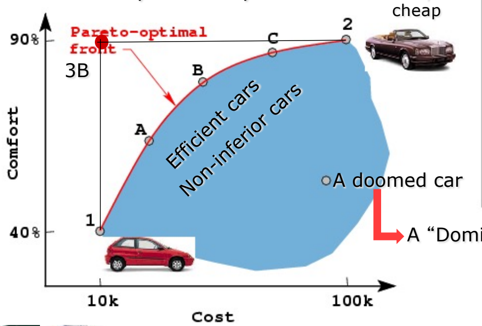
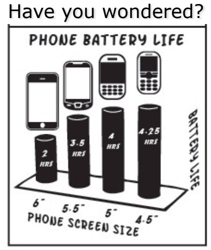
Multi-Objective Optimization: *Basics*

- Bueno, Bonito, Barato?

Good, nice, cheap



Have you wondered?



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Formally, as a Mathematical Programming Problem

- Multiple objectives, constraints, and variables

$$\begin{array}{ll} \text{Min/Max} & (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_M(\mathbf{x})) \\ \text{Subject to} & g_j(\mathbf{x}) \le 0 \\ & h_k(\mathbf{x}) = 0 \\ & \mathbf{x}^{(L)} \le \mathbf{x} \le \mathbf{x}^{(U)} \end{array} \rightarrow \boldsymbol{f}(\boldsymbol{x})$$

Optimal Solution — Solution — Point

- If x^* is *Pareto-optimal soln*., $\boldsymbol{f}(\boldsymbol{x}^*)$ is an *Efficient* pt.
- Set of all Pareto-optimal solutions ($\boldsymbol{x}^*$) is called *Pareto-optimal Set* (X_{Par})
- Set of all efficient points is called *Efficient Set* (Z)
- *Pareto-optimal front*: same as efficient set (EMO)

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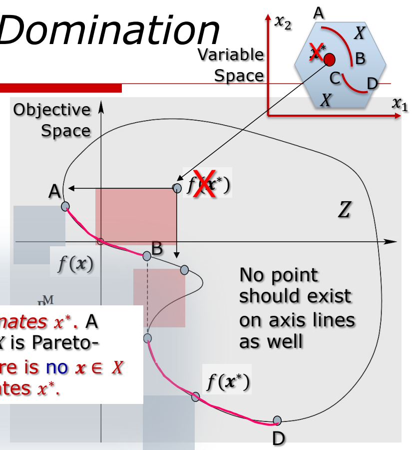
MOO Basics: *Domination*

- A solution $x^* \in X$ is Pareto-optimal if there is no $x \in X$ such that $f_i(x) \le f_i(x^*)$, $i = 1, \ldots, M$ and $f_j(x) < f_j(x^*)$ for some j
- Place top-right corner of paper on the point z^*
  - If no point exists on the paper, z^* is efficient

Then, x *dominates* x^*. A solution $x^* \in X$ is Pareto-optimal if there is no $x \in X$ which dominates x^*.



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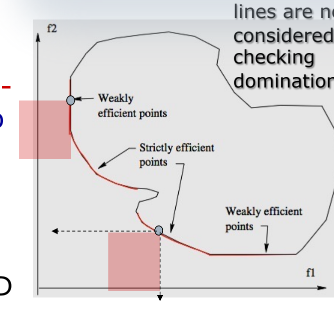
MOO Basics (cont.)

A solution $x^* \in X$ is weakly Pareto-optimal if there is no $x \in X$ which weakly dominates x^*

- *Weakly Efficient*
- A solution $x^* \in X$ is called weakly Pareto-optimal if there is no $x \in X$ such that $f_i(x) < f_i(x^*)$, for all $i = 1, \ldots, M$.
- Since less points dominate a point, ND set is larger

Points on axis lines are not considered for checking domination



Not much important for practical problems

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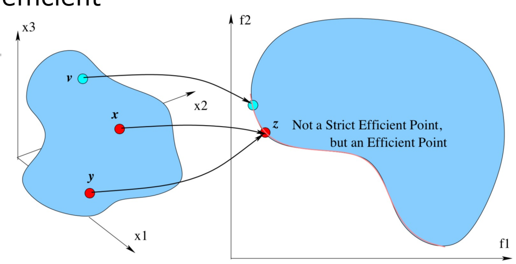
MOO Basics (cont.)

Note: There is no concept of *Strong-Domination*

- *Strictly Efficient*
  - Non-unique efficient points x^* are not strictly efficient

Multi-modal Pareto-optimal solutions are not strictly efficient



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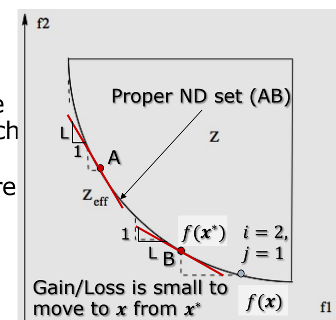
MOO Basics (cont.)

- *Properly Efficient*
- $x^* \in X$ is called Properly Pareto-optimal if it is Pareto-optimal and if there is a large number $L > 0$ such that for all i and $x \in X$ satisfying $f_i(x) < f_i(x^*)$ there exists an index j such that $f_j(x^*) < f_j(x)$ and

Trade-off = Gain/Loss = $\dfrac{f_i(\mathbf{x}^*) - f_i(\mathbf{x})}{f_j(\mathbf{x}) - f_j(\mathbf{x}^*)} \le L.$



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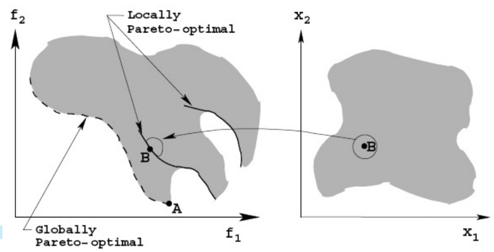
MOO Basics (cont.)

- *Locally Efficient*
- Domination check is restricted within a neighborhood (in decision space) of *B*



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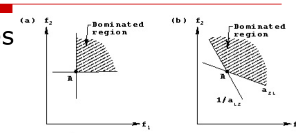
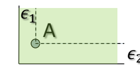
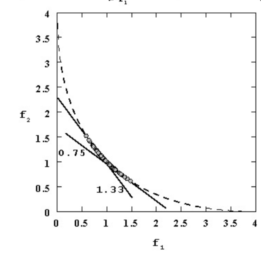
MOO Basics (cont.)

- Other Domination Principles
- *Cone-Domination*
- *Epsilon-Domination*





- One with larger number of objectives dominate the other
- Custom Domination principles possible



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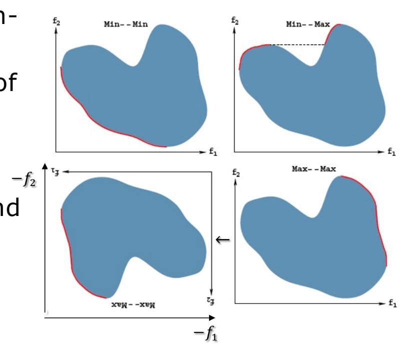
MOO Basics (cont.)

- Mixed minimization-maximization
1. Change definition of domination, or
2. Multiply Maximization objectives by -1 and treat all objectives to be minimized



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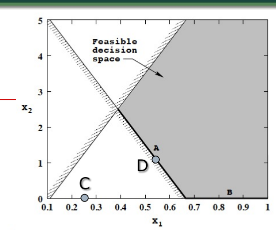
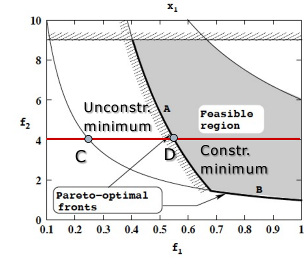
MOO Basics (cont.)

- *Constraint Handling:*
- Part of PO front may be active
- Penalty function approach:
  - $P_i(\boldsymbol{x}) = f_i(\boldsymbol{x}) + R_i CV(\boldsymbol{x})$, then Min $\{P_i(\boldsymbol{x})\}$
    - Results depends on R_i
  - Min $S(f_i(\boldsymbol{x}))$, subject to $g_j(\boldsymbol{x}) \leq 0$ for all j
    - S is weighted-sum, ASF or any other, discussed next





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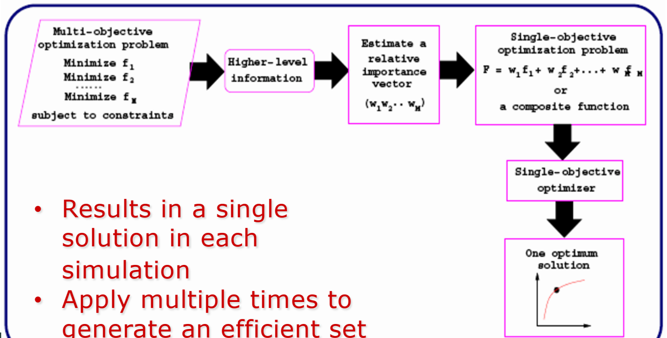
Classical MOO Principle



- Results in a single solution in each simulation
- Apply multiple times to generate an efficient set

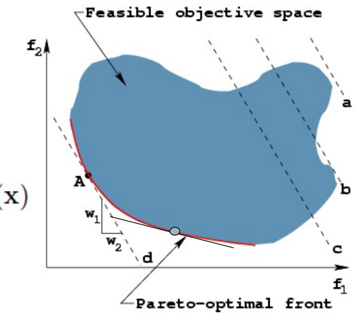
Classical Approach: *Weighted Sum Method*

- Construct a weighted sum of objectives and optimize

Minimize:

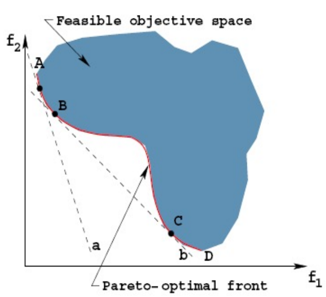
$$F_{w_1,w_2}(\mathbf{x}) = w_1 f_1(\mathbf{x}) + w_2 f_2(\mathbf{x})$$

- User supplies weight vector *w*



Difficulties Associated to Weighted-Sum Method

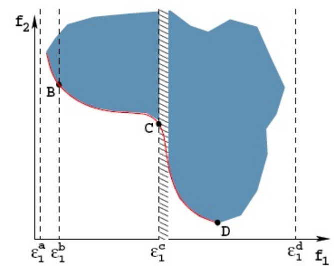
- Need to know **w**
- Non-uniformity in Pareto-optimal solutions
- Inability to find some Pareto-optimal solutions (those in non-convex region)
- However, a solution of this approach is always Pareto-optimal



ε-Constraint Method

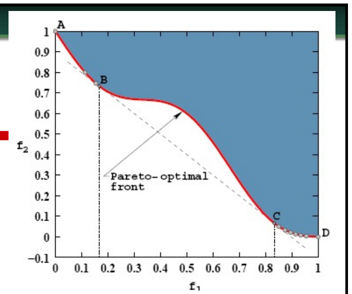
- Constrain all but one objective
- Need to know relevant **ε** vectors
- Non-uniformity in Pareto-optimal solutions
- However, any Pareto-optimal solution can be found with this approach

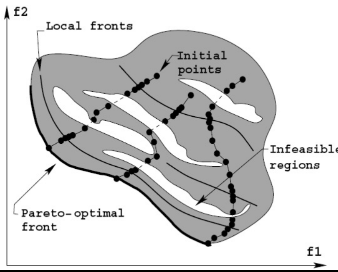
$$\text{Minimize} \quad f_\mu(\mathbf{x}),$$
$$\text{subject to} \quad f_m(\mathbf{x}) \le \epsilon_m, \quad m \ne \mu;$$



Difficulties with Classical Methods

- Need to run a single-objective optimizer many times
- Expect a lot of problem knowledge
- Multi-objective optimization treated as an application of single-objective optimization
- Absence of any parallel search





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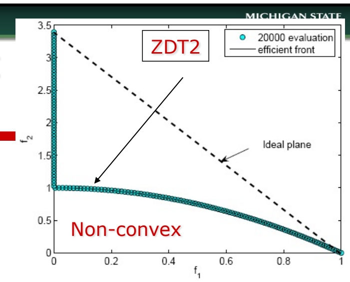
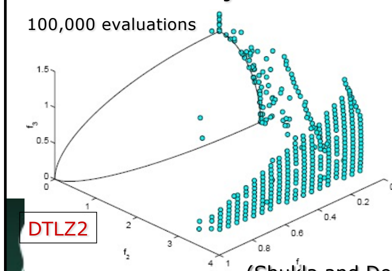
Normal Constraint Method Results

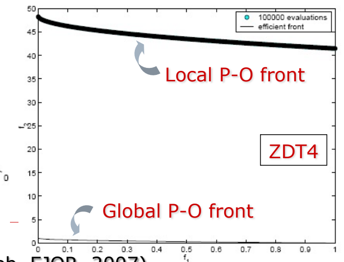
Difficulties:

- Weak P-O points
- Local P-O fronts
- More objectives



100,000 evaluations





(Shukla and Deb, EJOR, 2007)

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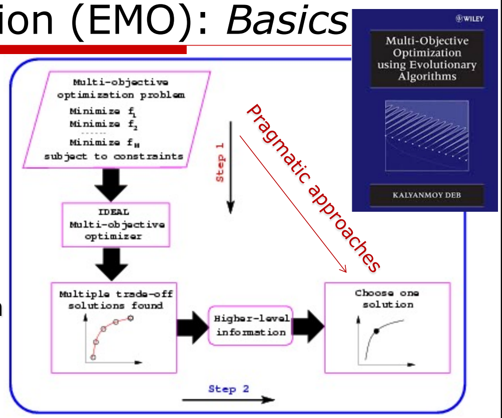
Evolutionary Multi-Criterion Optimization (EMO): *Basics*

Step 1 :

Find a set of Pareto-optimal solutions

Step 2 :

Choose one from the set



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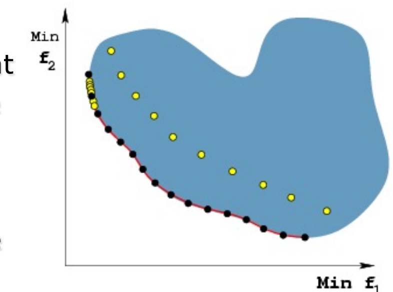
Three Goals in EMO

- Converge to the Pareto-optimal front
- Maintain as diverse a distribution as possible
- Preserve elites for better performance



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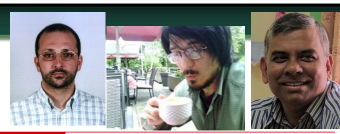
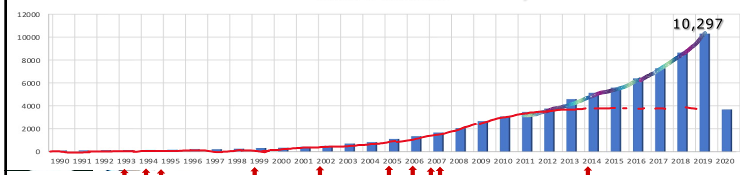
EMO: Past



- Early penalty-based approaches
- VEGA (1984)
- Goldberg's (1989) suggestion

- MOGA, NSGA, NPGA (1993-95) used Goldberg's suggestion
- Elitist EMO (SPEA, NSGA-II, PAES, MOMGA etc.) (1998 -- Present)



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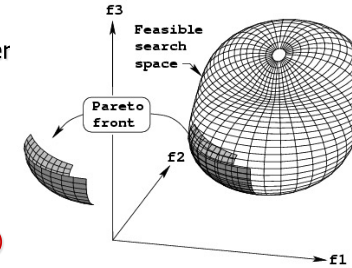
Elitist Non-dominated Sorting Genetic Algorithm (NSGA-II)

(Deb et al., IEEE TEC 2002)

- NSGA-II
  - Modular
  - No additional parameter
  - Fast
- Commercialization:
  - Heeds (NSGA-II like)
  - ModeFrontier (Estico)
  - iSIGHT (Engeneous)
  - VisualDoc (Vanderplatts)



Fast-Breaking Paper in Engineering by ISI Web of Science (Feb' 04), Thomson Citation Laureate Award 2006, Current Classic and Most Highly Cited Paper (40,000+ GS citations)

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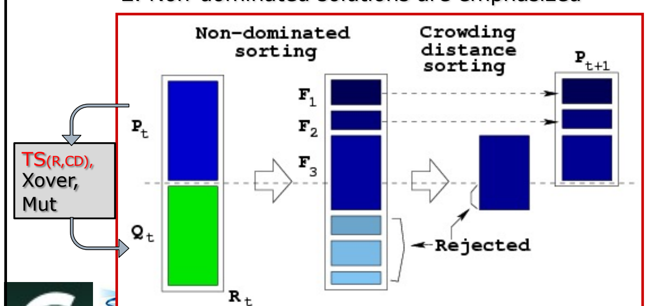
NSGA-II Procedure

$TS_{(R,CD)}(A,B)$:
if $R_A < R_B$, choose A
if $R_B < R_A$, choose B
else //A & B non-dominated
if $CD_A > CD_B$, choose A
if $CD_B > CD_A$, choose B
else choose rand(A,B)

1. Elites are preserved
2. Non-dominated solutions are emphasized



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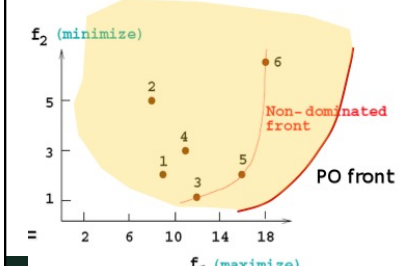
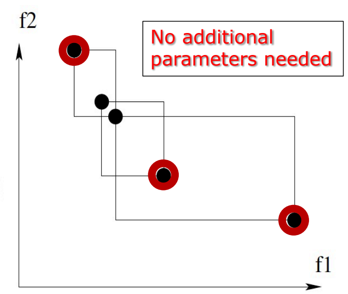
NSGA-II Procedure (cont.)

1. Emphasize for non-dominated points



2. Emphasize for less crowded points



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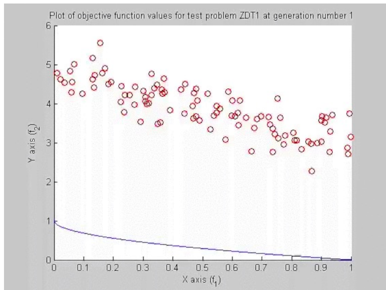
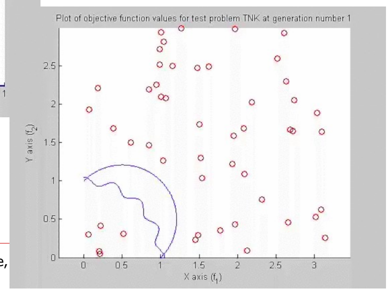
Simulation of NSGA-II



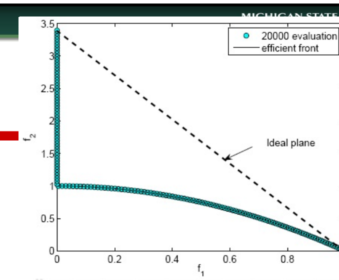
Unconstrained Problem ZDT1

Constrained Problem TNK

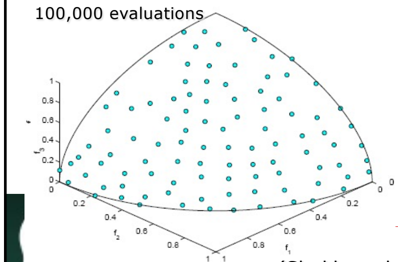


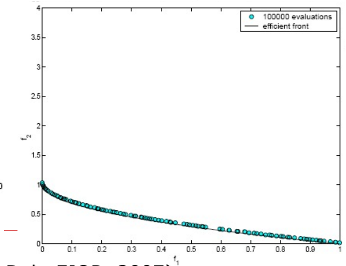
NSGA-II Head-to-head with NCM

- Population size=100
- Standard parameter setting
- Seems to work well



100,000 evaluations

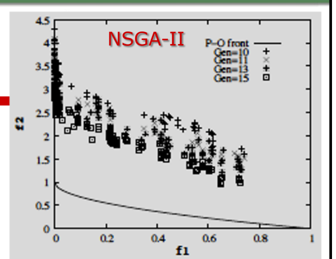


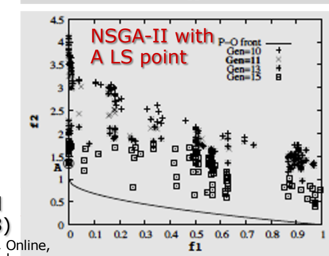


(Shukla and Deb, EJOR, 2007)

Why EMO Do So Well?

- Population approach suits well to find multiple solutions
- Niche-preservation methods can be exploited to find diverse solutions
- Implicit parallelism helps provide a parallel search
- Multiple applications of classical methods do not constitute a parallel search





(Sindhya, Deb, and Miettinen, PPSN-08)

Achievements in the Past: During 1993-2008

- Efficient EMO algorithms for 2-3 objectives demonstrated on test problems
  - Test problem suite (ZDT) helped early R&D
  - Advantage of EMO on 2-3 obj is overwhelming compared to 1-obj
  - Commercialization and spread to non-EC areas
- Limited practical applications
- What else to do?
  - Advanced Topics in EMO

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Progress During Immediate Past to Present (≥ 2009)

- EMO in many-objective optimization
- EMO + MCDM -- the whole story
- Visualization of EMO Solutions
- EMO to aid other problem solving
  - Multiobjectivization
- EMO for handling practicalities
- More efficient EMO Algorithms
- Theoretical EMO

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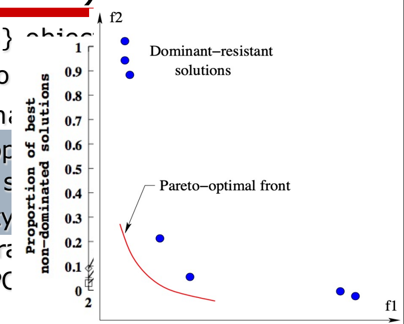
Evolutionary Many-Objective Optimization (EMO)

- Multi-objective: {2,3} objec
- Many-objective: >3 o
- EMO difficulties for ma
  1. Large fraction of pop
  2. Dominant resistant s
  3. Maintaining diversity
  4. Recombination opera
  5. Representation of PC more points
  6. Performance measures difficult to compute
  7. Visualization is difficult



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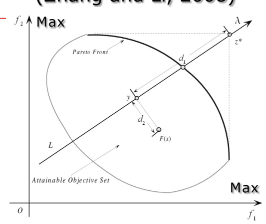
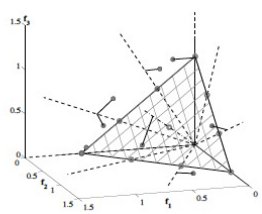
Decomposition Based EMO: MOEA/D

(Zhang and Li, 2008)

- Multiple reference lines
- Random association at first
- Points from neighboring (*T*) lines are mated
- Offsprings are associated with a line based on min.
  - $\text{PBI}(\mathbf{x}, \mathbf{w}) = d_1 + \theta d_2$.
  - $\text{TCH}(\mathbf{x}, \mathbf{w}, \mathbf{z}^*) = \max_{i=1}^{M} w_i |f_i(\mathbf{x}) - z_i^*|$
- Offspring can replace *r* parents
- No explicit selection operator





Original study to 2-3 obj.
Param: *T*, *θ*, *r*

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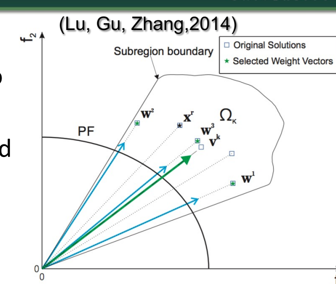
MOEA/D-M2M

(Lu, Gu, Zhang,2014)

- Objective space is divided into sub-regions
- MOEA/D or other EMO applied within sub-region
- Selection and recombination restricted to each sub-region
- Points are redistributed to the appropriate sub-region
- Later versions recombine across sub-regions with a probability
- Results are on 2 and 3 objectives



MEAN AND BEST OF IGD-METRIC VALUES OF MOEA/D-M2M, MOEA/D-DE, AND NSGA-II IN 20 INDEPENDENT RUNS FOR EACH TEST INSTANCE

IGD-metric	MOEA/D-M2M		MOEA/D-DE		NSGA-II	
Instance	best	mean	best	mean	best	mean
MOP1	**0.0151**	**0.0179**	0.2897	0.3239	0.2129	0.2206
MOP2	**0.0103**	**0.0118**	0.2167	0.2342	0.2103	0.2121
MOP3	**0.0116**	**0.0123**	0.4437	0.4798	0.2611	0.2660
MOP4	**0.0091**	**0.0102**	0.2662	0.2738	0.2745	0.2826
MOP5	**0.0153**	**0.0209**	0.2657	0.2925	0.2419	0.2442
MOP6	**0.0513**	**0.0526**	0.3039	0.3040	0.3040	0.3044
MOP7	**0.0623**	**0.0780**	0.3507	0.3507	0.3505	0.3505

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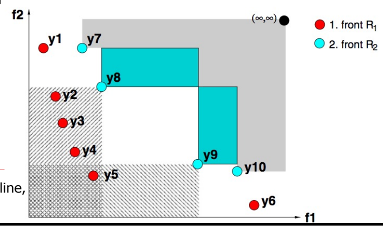
SMS-MOEA

(Beume, Naujoks and Emmerich, 2007)

- Steady-state EMO
- Multi-objective converted to a single-obj. optimization
- Every ND point is computed for its hypervolume contribution
- The worst one is deleted
- Original Study: 2 and 3-obj problems with success
- Use sample-based hypervolume metric for >3 objectives



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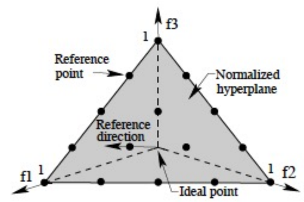
NSGA-III:

(Deb and Jain, 2014)

Step 0: Supply of Reference Points

- If no preference, use Das and Dennis's approach
- # pts.: $H = \binom{M+p-1}{p}$
- Else, supply a preferred set of reference points
- Points are given on the normalized hyper-plane
- Any other structured set of points can also be supplied



p=4, M=3, H=15

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NSGA-III:

(Deb and Jain, 2014)

Step 0: Supply of Reference Points

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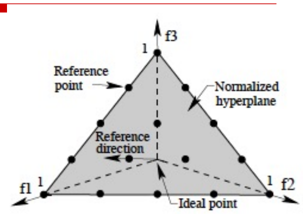
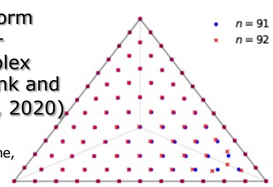


p=4, M=3, H=15

Uniform Unit-simplex (Blank and Deb, 2020)



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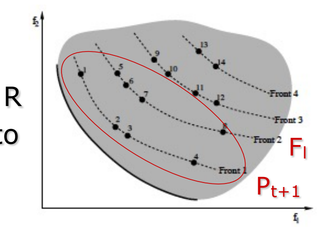
NSGA-III:

Step 1: Identification of Non-dominated Fronts

- Parent and offspring population combined to R
- Non-dominated sorting of R
- Collect and save fronts 1 to l to S, delete other fronts
- If |S|=N, P_{t+1} = S, go to next iteration
- Else, $P_{t+1} = \{F_1,\ldots,F_{l-1}\}$, remaining pts chosen from F_l



N=7

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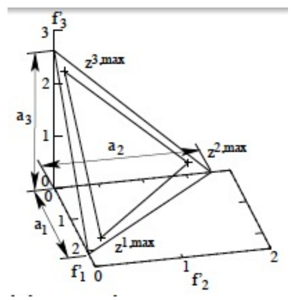
NSGA-III:

Step 2: Normalization of Population Members

- Identify ideal point of S
- Translate all members of S to make new ideal pt. as origin
- Identify extreme pts.:

$$ASF(\mathbf{x}, \mathbf{w}) = \max_{j=1}^{M} f_i'(\mathbf{x})/w_i, \quad \text{for } \mathbf{x} \in S_t$$

- Update with previous extreme pts.
- Normalize using ideal and extreme points obtained



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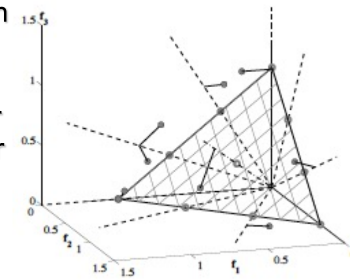
NSGA-III:

Step 3: Association of Population Members

- Reference line for each ref. pt. is found
- The ref. pt. having shortest perpendicular dist. from a S member is associated
- A reference point may have zero, one, or more than one S members associated



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NSGA-III:

Genetic Operators

- Selection Operator is not used.
- Recombination and mutation operators as before
- Use large value of distribution index of SBX
  - To create meaningful offspring

- No additional parameter needed, like in NSGA-II, unlike in MOEA/D

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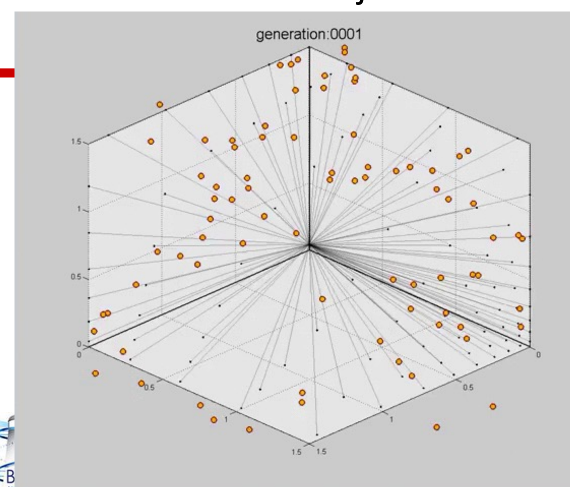
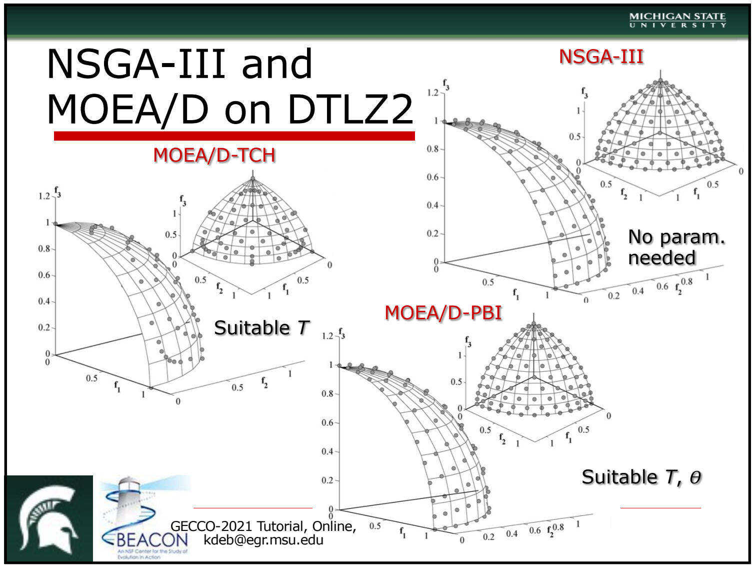
NSGA-III Simulation on 3-Obj. Problem

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NSGA-III and MOEA/D on DTLZ2
NSGA-III
MOEA/D-TCH
No param. needed
Suitable T
MOEA/D-PBI
Suitable T, θ
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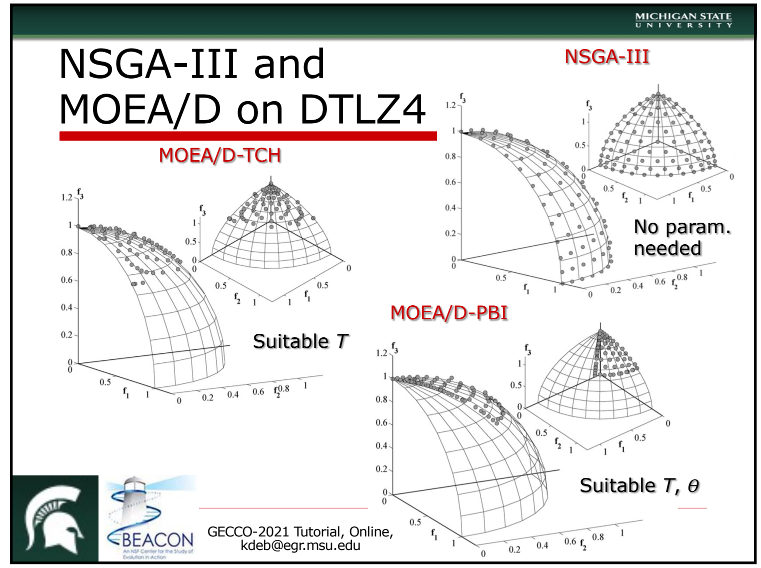
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NSGA-III and MOEA/D on DTLZ4
NSGA-III
MOEA/D-TCH
No param. needed
Suitable T
MOEA/D-PBI
Suitable T, θ
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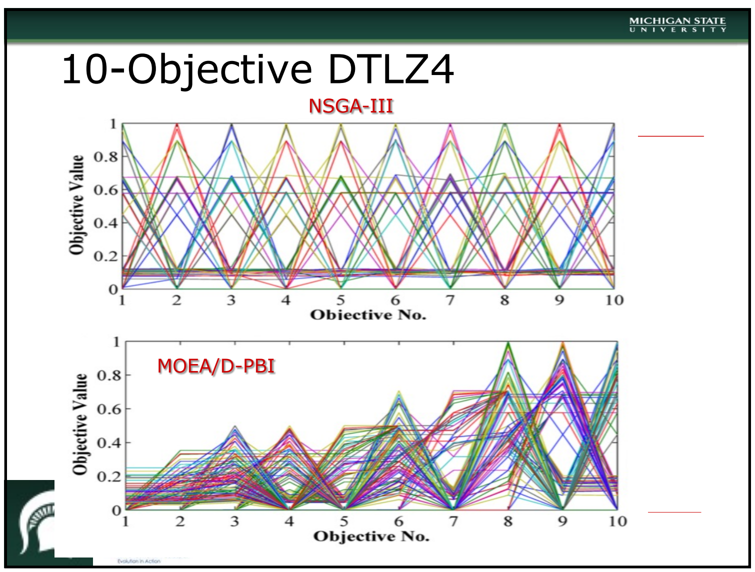
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10-Objective DTLZ4
NSGA-III
Objective Value
Objective No.
MOEA/D-PBI
Objective Value
Objective No.

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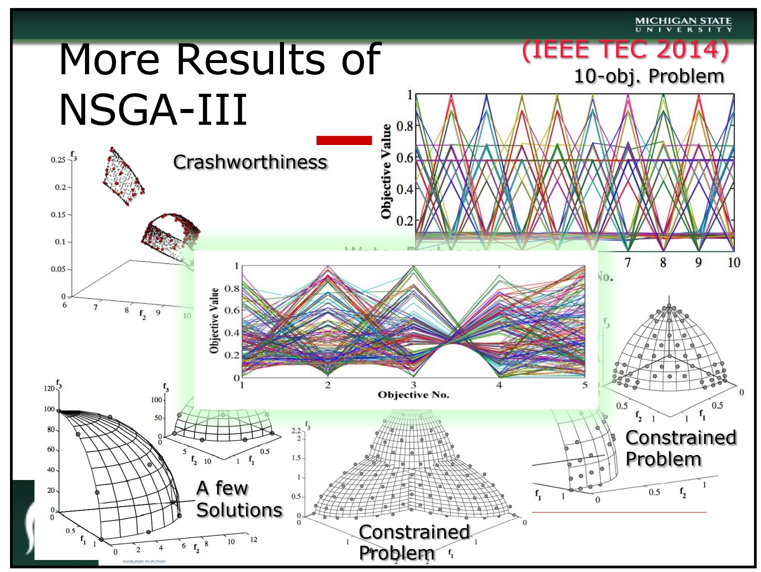
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More Results of NSGA-III
(IEEE TEC 2014)
10-obj. Problem
Crashworthiness
Objective Value
Objective Value
Objective No.
A few Solutions
Constrained Problem
Constrained Problem

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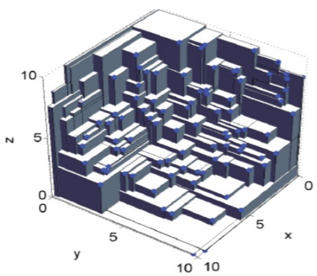
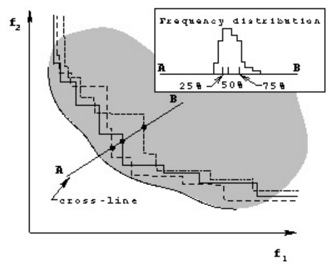
Metrics for Convergence and Diversity

Hypervolume



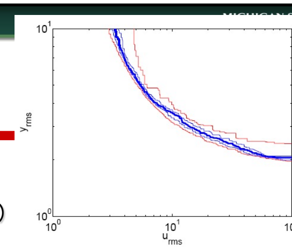
Attainment Surface Method

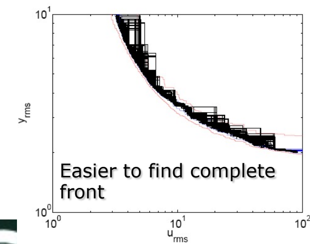


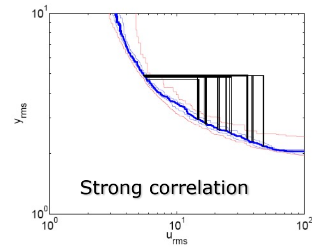
Attainment Surface Methods

- Positive and negative relationships

Fonseca (2005; 2007)

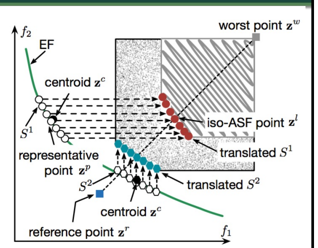


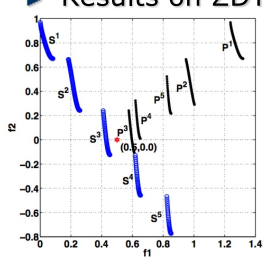




Reference Point Based HV/IGD

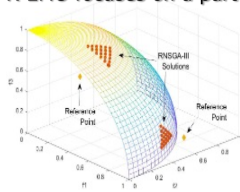
- Move points on the reference line and compute HV
- Results on ZDT3





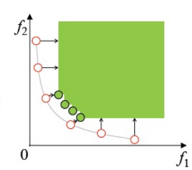
(a) Population distribution.

R-EMO focuses on a part



(b) R-NSGA-III (Vesikar, Deb and Blank, 2018)

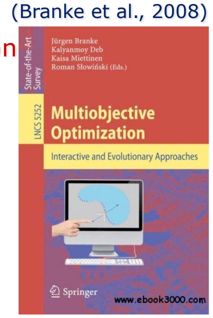
IGD+:
(Ishibuchi et al., 2015)



EMO and Decision-Making

- Finding a P-O set (using EMO) is half the story
- How to choose one preferred solution (MCDM)
- A-priori approach:
  - First MCDM, then EMO
- A-posteriori approach:
  - First EMO, then MCDM
- Interactive approach:
  - MCDM during EMO

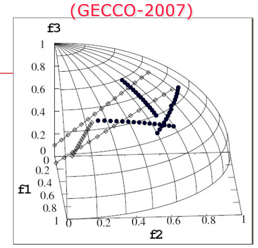
(Branke et al., 2008)



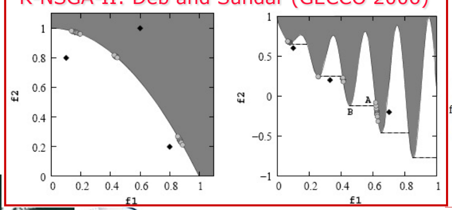
Making Decisions: *A Priori or A Posteriori*

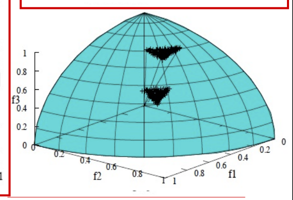
- Ranking based on closeness to each reference point or a reference direction

RD-NSGA-II: Deb and Kumar (GECCO-2007)



R-NSGA-II: Deb and Sundar (GECCO 2006)

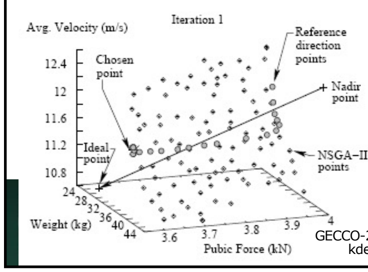




'Light Beam' Approach in CEC-07

Example: Car Side Impact Problem

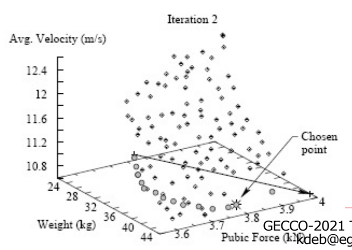
- Three objectives, 10 constraints, seven variables
- Utility: Min. avg. force at abdomen and pubic area
- q^0=nadir point=(42.69,4.00,12.44)
- g^1=ideal point=(24.37,3.59,10.61)
- 25 points -> q^1=(35.95,3.56,11.53)

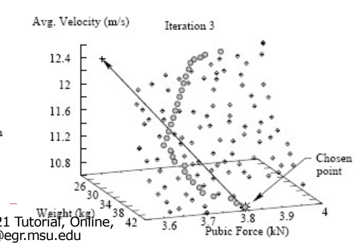


- Avg. vel (f_3) smaller
- g^2=(42.69,4.00,10.61)
- RD: q^2 to g^2
- 15 points

Second and Third Iterations

- q^2=(40.98,3.81,10.61), f_3 is reduced
- Reduce f_1 and f_2: g^3=(24.37,3.59,12.44)
- q^3=(40.92,3.81,10.61)
- Consider q^2 and q^3 close and terminate
- Declare x-vector





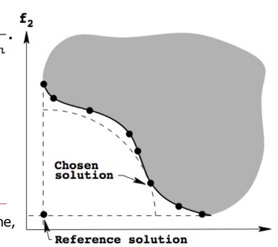
A-Posteriori Approaches

- Any of the a priori approaches can be applied after a set of non-dominated points are found
- Compromise Programming:

l_p-metric: $$d(\mathbf{f},\mathbf{z}) = \left(\sum_{m=1}^{M} |f_m(\mathbf{x}) - z_m|^p\right)^{1/p},$$

Tchebycheff metric: $$d(\mathbf{f},\mathbf{z}) = \max_{m=1}^{M} \frac{|f_m(\mathbf{x}) - z_m|}{\max_{\mathbf{x}\in\mathcal{S}} f_m(\mathbf{x}) - z_m}.$$

- Need a reference point
  - Usually the ideal point
- Quite common in practice



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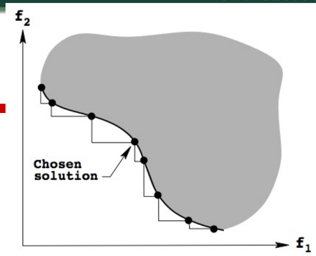
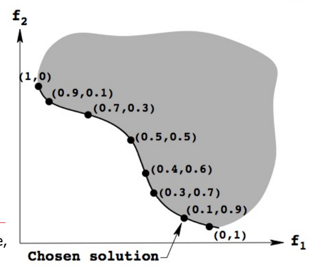
A Posteriori Approaches (Cont.)

- Trade-off Approach
  - Recent applications
- Pseudo-weight Approach:

$$w_i = \frac{(f_i^{max} - f_i(\mathbf{x}))\,/\,(f_i^{max} - f_i^{min})}{\sum_{m=1}^{M} (f_m^{max} - f_m(\mathbf{x}))\,/\,(f_m^{max} - f_m^{min})}$$

  - Choose a solution close to desired weight combination





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Visualization Methods in EMO

- Bar Charts
- Scatter Plots
- Multi-way Dot Plots
- Table Lens Plots
- Heat Maps
- Parallel Coordinate Plots (PCP)
- Level Diagrams and Hyper Radial Visualization (HRV)

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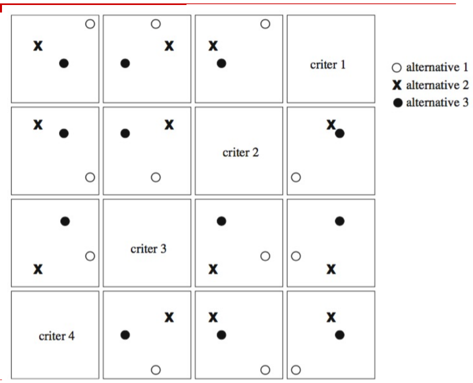
Scatter Plot

- M choose 2 pair-wise combinatio ns

(Chambers and Kleiner, 1982)



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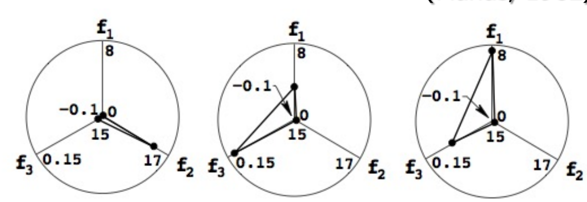
Star-Coordinate Method

- Used in some softwares
- Still cannot get a good idea of trade-off

(Manas, 1982)



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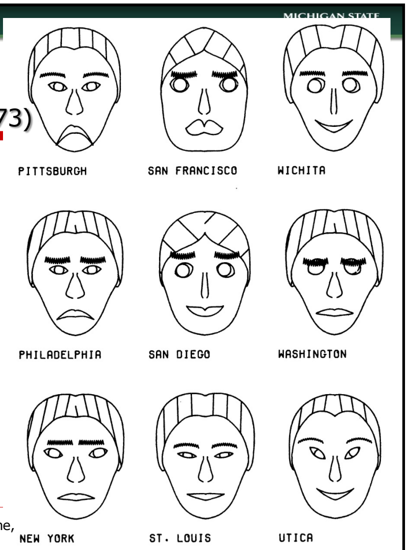
Chernoff Faces (Chernoff, 1973)

- 16 features represent 16 objectives
- Pittsburgh: High pollution (mouth)
- Wash: High prop of non-white pop. (pos. of eyebrow)
- San Fransisco: Low density of pop (eye separated)



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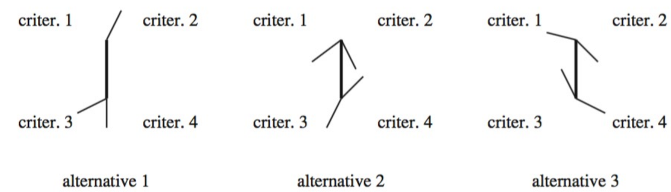
Stick Figure

- Angles (and length) of sticks represent objectives



(Pickett and Grinstein, 1988)

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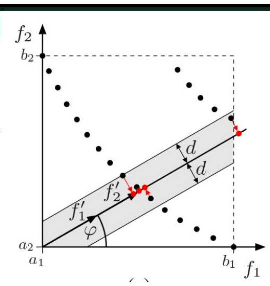
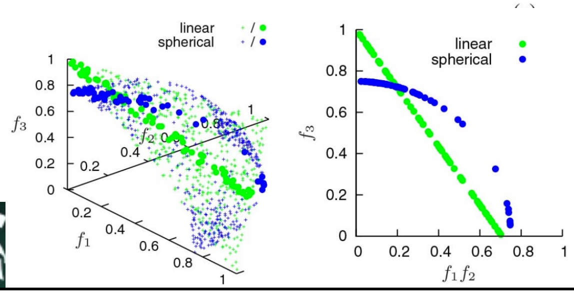
Prosection Method (Tusar and Filipic, 2014)

- Make a slice along M-dim PO front and project on a hyperplane

$m\mathrm{D}(\boldsymbol{a}, f_i f_j, \varphi, d)$





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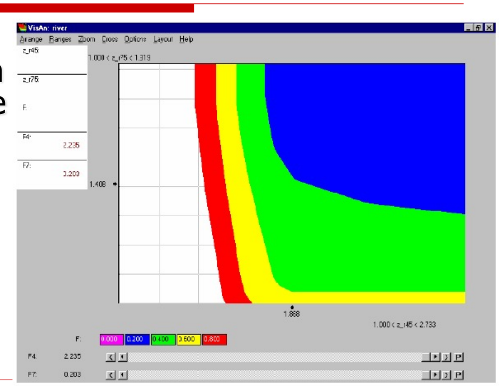
Decision Maps (Lotov, 2004)

- Three objective in prominence
- Others as scroll bars
- Requires pre-processing



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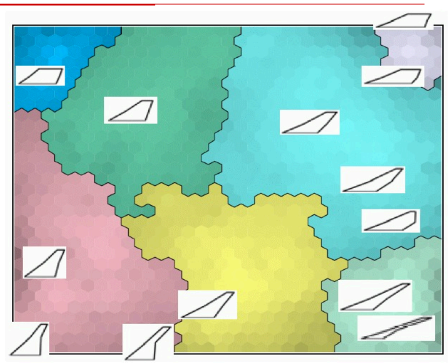
Self-Organizing Maps

- Design space is divided based on similarity in variables

(Kohonen, 2001)



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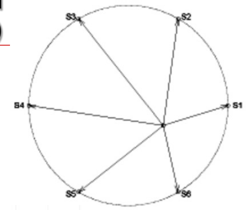
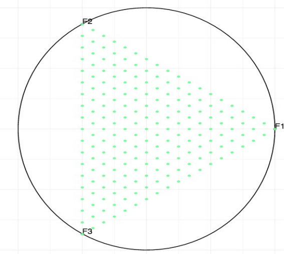
Radial Coordinate Visualization (RadViz)

(Hoffman and Grindstein, 1997)

- A puck is in equilibrium from M points on the circle with stiffness prop. to obj values





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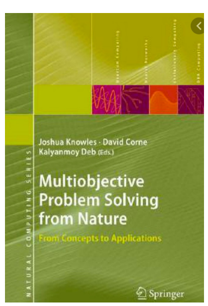
Multiobjectivization:

Solving Problems Using MO Principle

- Constrained handling
  - Constraint violations as additional objectives
- Multimodal problems
- Bloating in Genetic Programming (Blueler et al, 2001)
- Diversity preservation in EAs (Jensen, 2003, Abbas and Deb, 2003)
- Fuzzy clustering methods
- Goal programming



(Knowles, Corne & Deb, 2008)

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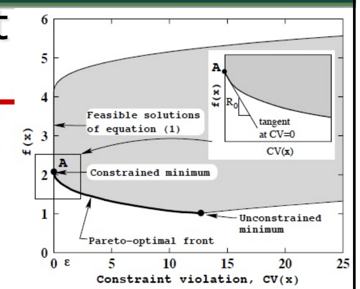
1-obj. Constraint Handling

minimize
subject to

minimize
minimize

- Pose as a two-obj problem
- Compare penalty-based approach with weighted-sum approach



Penalty Function Approach:

$$P(\mathbf{x}, R) = f(\mathbf{x}) + R \cdot \mathrm{CV}(\mathbf{x}),$$
$$= f_2(\mathbf{x}) + R f_1(\mathbf{x}),$$

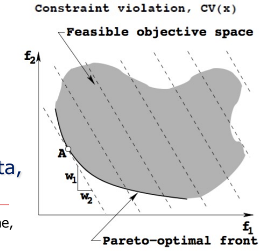
Bi-objective Approach:

$$\text{minimize} \quad F_{w_1,w_2}(\mathbf{x}) = w_1 f_1(\mathbf{x}) + w_2 f_2(\mathbf{x}).$$

Equating the two:

$$w_1 = R \text{ and } w_2 = 1.$$

(Deb and Datta, EO, 2012)



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EMO + Classical Penalty Based Approach

- EMO to get R
- Classical penalized approach to find a local solution
- Improvements of one or two-order in standard test problems

Prob.	Zavala, Aguirre & Diharce [52]			Takahama & Sakai [45]			Brest [6]			Proposed Hybrid Approach		
	Best	Median	Worst	Best	Median	Worst	Best	Median	Worst	Best	Median	Worst
g01	80,776	90,343	96,669	18,594	19,502	19,917	51,685	55,211	57,151	**2,630**	**3,722**	**4,857**
g02	87,419	93,359	99,654	1,08,303	114347	1,29,255	1,75,090	2,26,789	2,53,197	**26,156**	**50,048**	**63,536**
g04	93,147	1,03,308	1,109,15	12,771	13,719	14,466	56,730	62,506	67,383	**1,210**	**1,449**	**2,295**
g06	95,944	1,09,795	1,30,293	5,037	5,733	**6,243**	31,410	34,586	37,033	**1,514**	**4,149**	11,735
g07	1,14,709	1,38,767	2,08,751	60,873	67,946	75,569	1,84,927	1,97,901	2,21,866	**15,645**	**30,409**	**64,732**
g08	2,270	4,282	5,433	**621**	**881**	**1,173**	1,905	4,044	4,777	822	1,226	2,008
g09	94,593	1,03,857	1,19,718	19,234	21,080	21,987	79,296	89,372	98,062	**2,732**	**4,850**	**5,864**
g10	1,09,243	1,35,735	1,93,426	87,848	92,807	**1,07,794**	2,03,851	2,20,676	2,64,575	**7,905**	**49,102**	1,80,446
g12	482	6,158	9,928	2,901	4,269	5,620	**364**	6,899	10,424	496	**504**	**504**
g18	97,157	1,07,690	1,24,217	46,856	57,910	60,108	1,39,131	1,69,638	1,91,345	**4,493**	**7,267**	**10,219**
g24	11,081	18,278	6,33,378	1,959	2,451	**2,739**	9,359	12,844	14,827	**1,092**	**1,716**	2,890

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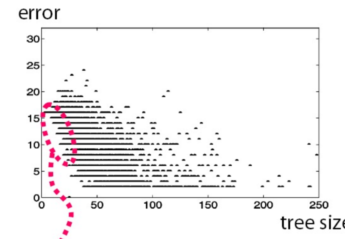
Reducing Bloating in GP

- Bleuler et al., (2001)
- Find small-sized programs with small error
- Minimization of Size of Program as second objective



Keep and optimize small trees (potential building blocks)

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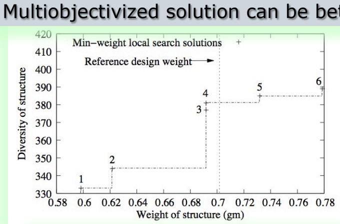
EMO to Explore Design Space

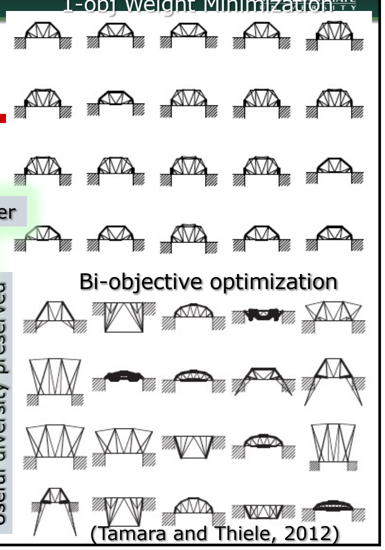
- Use of additional objectives for a reason
- Bi-objective optimization

Multiobjectivized solution can be better



(Sharma, Deb, Kishore, 2013)

1-obj Weight Minimization



Bi-objective optimization

Useful diversity preserved

(Tamara and Thiele, 2012)

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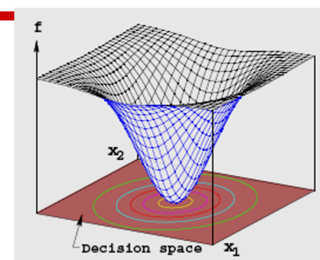
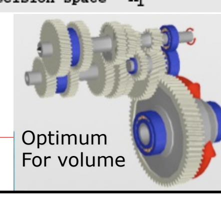
Innovization: Learning from Trade-off Solutions

- Often, one optimum x*
- x* minimizes f(x) subject to satisfaction of some constraints
- *Sensitivity analysis* provides neighborhood information
- Not much can be learned from one solution





Optimum For volume

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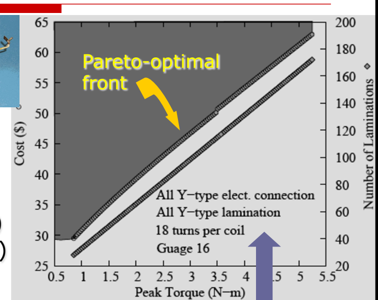
Case Studies of Manual *Innovization*: *Brushless DC Permanent Magnet Motor Design for Cost and Peak Torque*

- Five variables (all discrete), three constraints
- Non-convex, disconnected P-O fronts
- *Innovization*:
  - Connection: Y (betn. Y & Δ)
  - Lamination Type: Y (X, Y, Z)
  - 1 out of 16 wire guages
  - 18 turns per coil (10,80)
  - More peak torque by adding linearly more laminations



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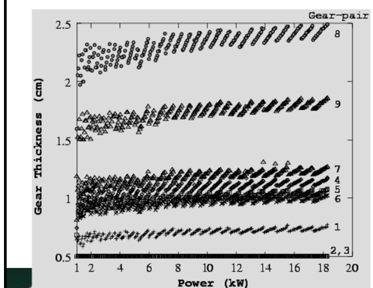
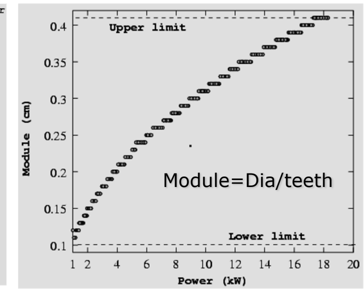
Gear-box Design: Innovized Principles

- Module (discrete) varies proportional to square-root of power
- Keep other 28 variables more or less the same





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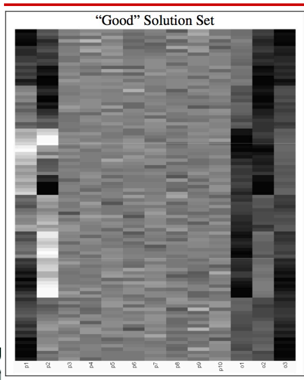
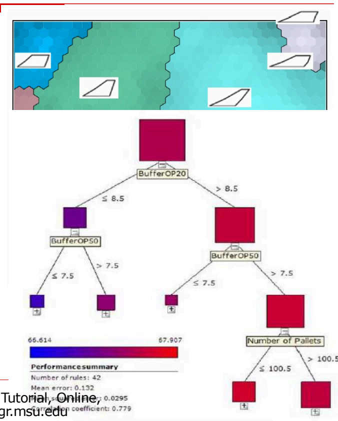
Heatmap, SOM and Decision Tree From Pareto-Optimal Set





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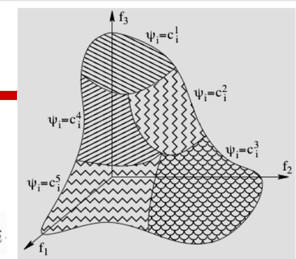
Automated Innovization

- Rules of type: $\psi_i(\mathbf{x}, \mathbf{f}(\mathbf{x}), \mathbf{g}(\mathbf{x})) = c_i.$
- Currently, limited to $\psi_i(\phi(\mathbf{x})) \equiv \Pi_{j=1}^{N} \phi_j(\mathbf{x})^{b_{ij}} = c_i$
- Solve (m data points):



(Bandaru and Deb, 2010, EO)

$$\begin{aligned} &\text{Minimize} \quad \left(number\ of\ clusters + unclustered\ points + \sum_{clusters} c_v \right), \\ &\text{Subject to} \quad 1 \le d_i \le m, \\ &\qquad unclustered\ points \le 0, \\ &\qquad -1 \le b_{ij} \le 1\ \forall j, \\ &\qquad |b_{ij}| \ge 0.1\ \forall j, \\ &\qquad d_i \text{ is an integer and } b_{ij}\text{'s are real.} \end{aligned}$$

Coeff. of variance

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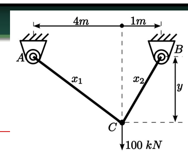
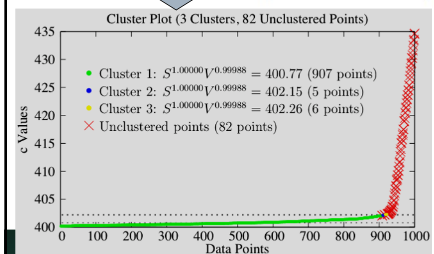
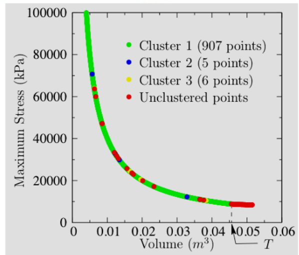
Truss Design



- Obtained Rules (independent applications):

$$SV = 400.77, \quad \frac{x_1}{V} = 0.1105, \quad \frac{x_2}{V} = 0.2236, \quad \frac{x_2}{x_1} = 1.9838$$





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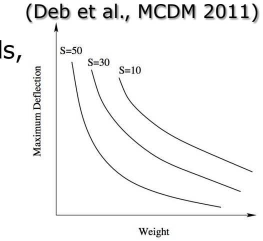
Higher-Level *Innovization*

(Deb et al., MCDM 2011)

- Over different parameter settings
  - Material properties, load, bounds, resources
- Over different variable sizes and types
  - Continuous to discrete
- Over multi-modal solutions
- Over different constraint combinations
- More possibilities



Procedure:
- Multiple fronts put together -> straightforward
- Perform *innovization* task

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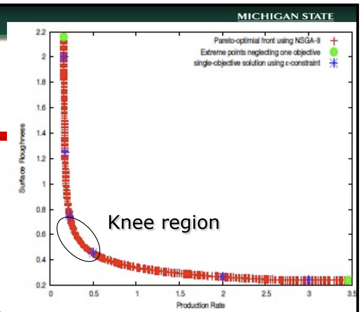
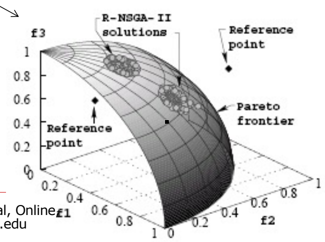
Lower-Level *Innovization*

- Knee region
- Over Preferred PO solutions
  - Reference point based solutions, weight based solutions
- Over specified values of objective or constraints or variable boundaries
- Over some fixed values of variables





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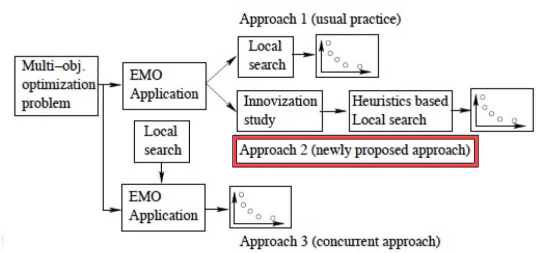
Innovization to Speed-up Optimization

(Deb and Datta, 2013 EO)

- Innovized principles as heuristics for local searches for a further EMO run
- A metal-cutting problem



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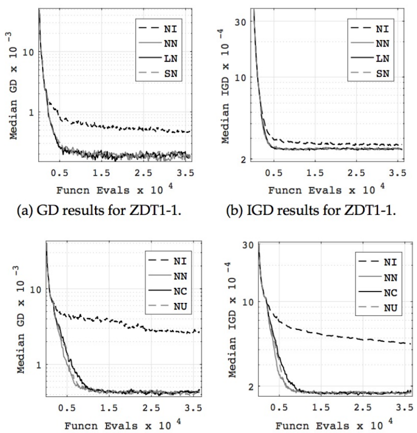
New Results on Innovization Based EMO Convergence

(Gaur and Deb, CEC-2017)



(a) GD results for ZDT1-1. (b) IGD results for ZDT1-1.

(a) GD results for ZDT1-2. (b) IGD results for ZDT1-2.

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EMO for Handling Practicalities

- Metamodeling based EMO
- Uncertainty handling EMO
- Distributed computing in EMO
- Objective reduction in EMO
- Dynamic EMO
- Bilevel EMO
- Etc.

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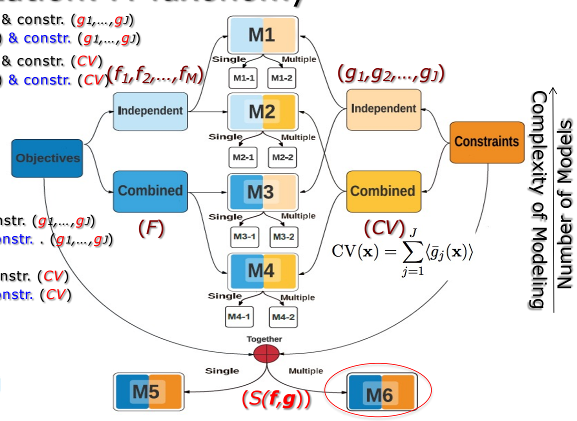
Metamodeling in Multi-objective Optimization: A Taxonomy

M1-1: ASF($f_1,\ldots,f_M$) & constr. ($g_1,\ldots,g_J$)
M1-2: MOO($f_1,\ldots,f_M$) & constr. ($g_1,\ldots,g_J$)
M2-1: ASF($f_1,\ldots,f_M$) & constr. (CV)
M2-2: MOO($f_1,\ldots,f_M$) & constr. (CV)

M3-1: ASF(F) & constr. ($g_1,\ldots,g_J$)
M3-2: MMO(F) & constr. . ($g_1,\ldots,g_J$)

M4-1: ASF(F) & constr. (CV)
M4-2: MMO(F) & constr. (CV)

M5: ASF(F + CV)
M6: MMO(F + CV)



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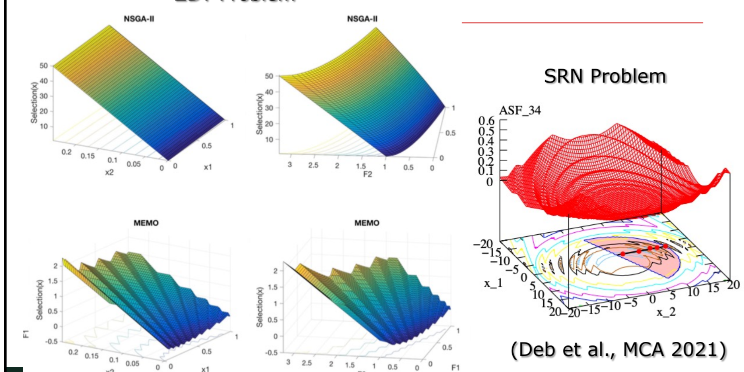
Selection Function:

ZDT Problem



(Deb et al., MCA 2021)

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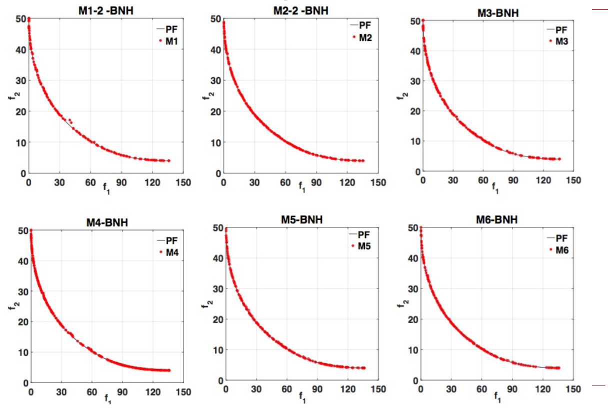
First Results

(Indv. Frameworks)

(Deb et al., EMO-17)



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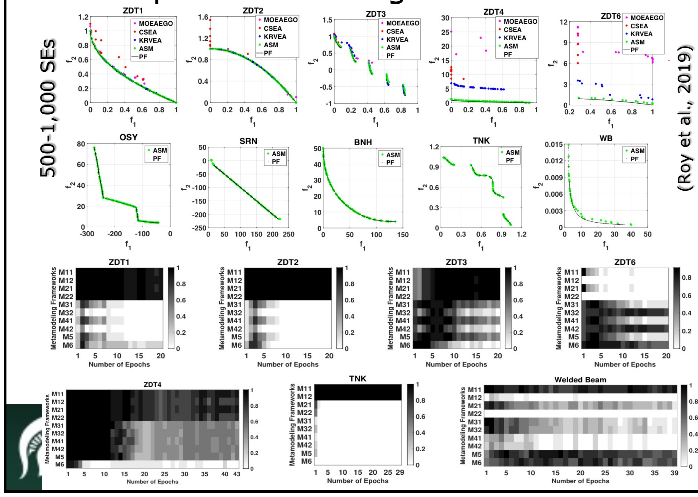
Adaptive Switching of Frameworks

500-1,000 SEs

(Roy et al., 2019) COIN Rep. 2019002



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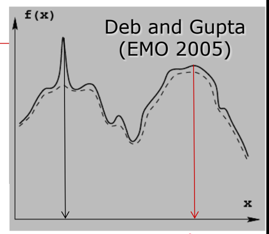
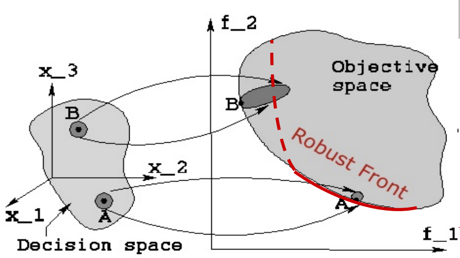
Robust EMO:

Handling uncertainties in variables and parameters

- Parameters are uncertain and sensitive to implementation
  - Find robust, instead of optimal, solution





- Robustness can be used as DM tool
- Robust front can be identified

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Multi-Objective Robust Solutions of Type I and II

- Similar to single-objective robust solution of type I

$$\begin{aligned} &\textit{Minimize} && (f_1^{\rm eff}(\mathbf{x}), f_2^{\rm eff}(\mathbf{x}), \ldots, f_M^{\rm eff}(\mathbf{x})), \\ &\textit{subject to} && \mathbf{x} \in \mathcal{S}, \end{aligned}$$

- Type II

$$\begin{aligned} &\textit{Minimize} && \mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_M(\mathbf{x})), \\ &\textit{subject to} && \frac{\|\mathbf{f}^{\rm p}(\mathbf{x}) - \mathbf{f}(\mathbf{x})\|}{\|\mathbf{f}(\mathbf{x})\|} \leq \eta, \\ & && \mathbf{x} \in \mathcal{S}. \end{aligned}$$

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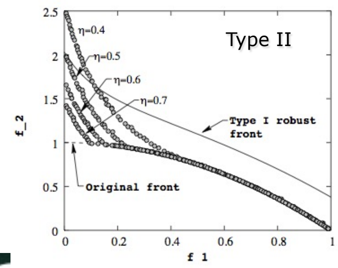
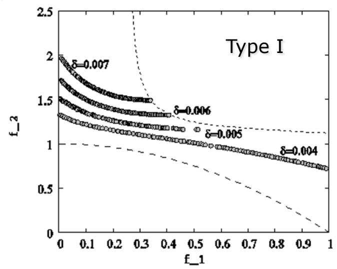
Robust Frontier for Two Objectives

- Identify robust region
- Allows a control on desired robustness





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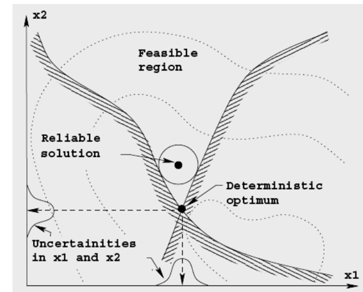
Reliability-Based Optimization:

Making designs safe against failures

- Deterministic optimum is not usually reliable
- Reliable solution is an interior point
- Chance constraints with a given reliability

Minimize $\mu_f + k\sigma_f$
Subject to $Pr(g_j(x)\geq 0) \geq \beta_j$
β_j is user-supplied



Deb et al. (EMO 2005)

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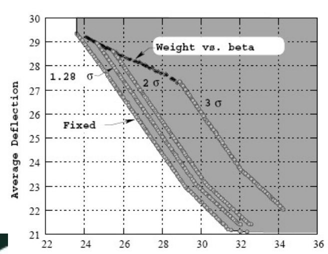
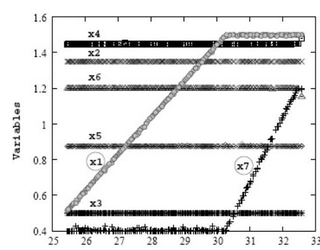
Multi-Objective Reliability-Based Optimization

- Reliable fronts show rate of movement
- What remains unchanged and what gets changed!





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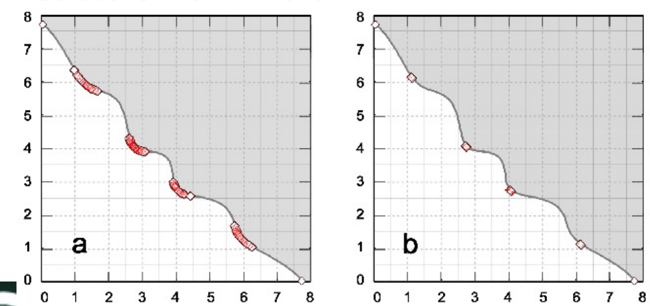
Finding Knee Solutions

Branke et al. (2004): Identifying knee-like solutions in a ND front



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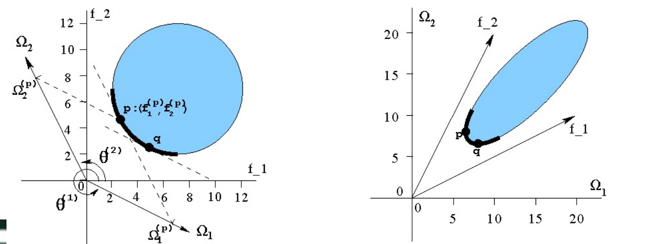
Distributed Computing of Pareto-Optimal Set

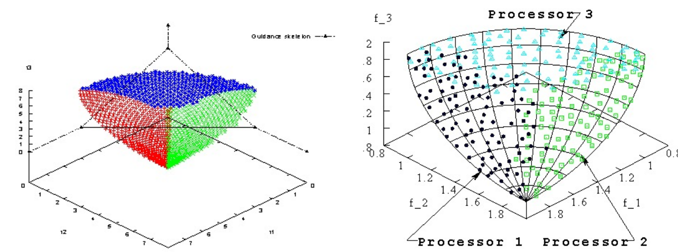
Deb, Zope & Jain (EMO-2003)

- Guided domination concept to search different parts of Pareto-optimal region
- Distributed computing of different parts



Distributed Computing: A Three-Objective Problem

- Spatial computing, not temporal



Objective Reduction

- Identify redundant objectives
- EMO+PCA in iterations

Iter.1

Iter. 1 : PCA-1 (58.83 % variance)		f_7	f_{10}
PCA-2 (28.26 % variance)	f_1		
PCA-3 (06.53 % variance)		f_8	
PCA-4 (03.27 % variance)		f_8	

10-objective DTLZ5 problem

	f_1	f_7	f_8	f_{10}
f_1	+	-	+	-
f_7	-	+	+	-
f_8	+	+	+	-
f_{10}	-	-	-	+

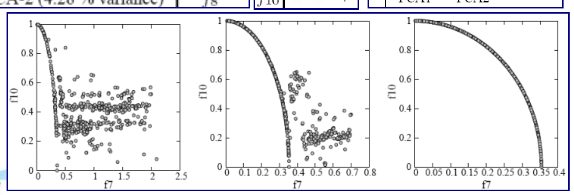
Iter.2

Iter. 2 : PCA-1 (94.58 % variance)	f_7	f_{10}
PCA-2 (4.28 % variance)	f_8	

	f_7	f_8	f_{10}
f_7	+	+	-
f_8	+	+	-
f_{10}	-	-	+

	e1:0.9458 e2:0.0428		
f_7	+0.543	-0.275	c7=0.5253
f_8	+0.457	+0.672	c8=0.4610
	PCA1	PCA2	

Saxena and Deb (CEC-2006, EMO-2007, CEC-2007)



EMO's Future

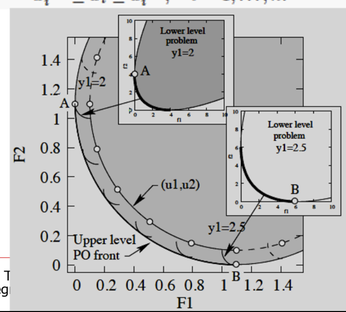
(Some Pilot Work Done Before)

- Handling further practicalities
  - Hierarchical problem solving
  - Multi-modal PO sets
  - Lexicographic problems
  - Massive (>20) objectives
- Theoretical developments
- More efficient many-obj algorithms
- Interactive EMO-MCDM
- EMO to AI and ML applications

Multi-Objective Bilevel Programming (Deb and Sinha, ECJ-2010)

- Upper level solution is feasible only if it is a lower level PO solution
- Often appears in engineering problems to deal with stability, equilibrium etc.
- NSGA-II in both levels

$$\min_{(\mathbf{x}_u,\mathbf{x}_l)} \mathbf{F}(\mathbf{x}) = (F_1(\mathbf{x}),\ldots,F_M(\mathbf{x})),$$
$$\text{s.t.} \quad \mathbf{x}_l \in \operatorname{argmin}_{(\mathbf{x}_l)} \left\{ \mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}),\ldots,f_m(\mathbf{x})) \middle| \mathbf{g}(\mathbf{x}) \geq \mathbf{0}, \mathbf{h}(\mathbf{x}) = \mathbf{0} \right\},$$
$$\mathbf{G}(\mathbf{x}) \geq \mathbf{0}, \mathbf{H}(\mathbf{x}) = \mathbf{0},$$
$$x_i^{(L)} \leq x_i \leq x_i^{(U)}, \quad i = 1,\ldots,n.$$



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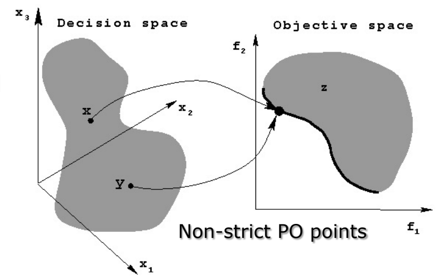
Multi-Modal EMOs

- Different solutions having identical objective values
- Multi-modal Pareto-optimal solutions: Design, Bioinformatics
- Find multiple solutions having identical objective values
- Modified crowding approach in NSGA-II



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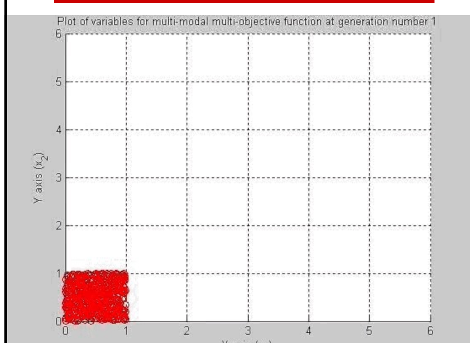
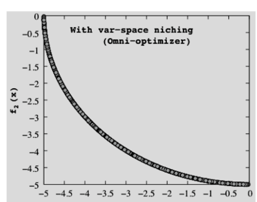
Multi-Modal Multi-Objective Problem: (Omni-Optimizer, Tiwari and Deb, EJOR-08)



Each part produces An identical front



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Theoretical Developments

- KKT Proximity Measure (KKTPM) for convergence
- Performance Measures
  - Hypervolume (exact and sample-based)
  - Attainment surfaces
  - R-HV for reference point-based EMO
- Other theoretical studies

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KKT Proximity Metric

Treat ASF as single-obj. problem

- Solve and find optimal ϵ_k*

$$\begin{aligned} \text{Minimize}_{(\epsilon_k, x_{n+1}, \mathbf{u})} \quad & \epsilon_k + \sum_{j=1}^{J} \left(u_j g_j(\mathbf{x}^k)\right)^2, \\ \text{Subject to} \quad & \|\nabla F(\mathbf{y}) + \sum_{j=1}^{J+M} u_j \nabla G_j(\mathbf{y})\|^2 \leq \epsilon_k, \\ & \sum_{j=1}^{M+J} u_j G_j(\mathbf{y}) \geq -\epsilon_k, \\ & u_j \geq 0, \quad j = 1, 2, \ldots, (M+J), \\ & -\epsilon_k \leq 0, \\ & -x_{n+1} \leq 0. \end{aligned}$$

1. Relax compl. slackness cond.
2. Add a penalty

- Define KKTPM:

Use Matlab's fmincon() to solve it
- 1 linear and 1 quadratic constraints

$$\text{KKT Proximity Measure}(\mathbf{x}^k) = \begin{cases} \epsilon_k^*, & \text{if } \mathbf{x}^k \text{ is feasible,} \\ 1 + \sum_{j=1}^{J} \langle g_j(\mathbf{x}^k) \rangle^2, & \text{otherwise.} \end{cases}$$

KKTPM Calculator: http://haithamseada.com/kktpm-calculator

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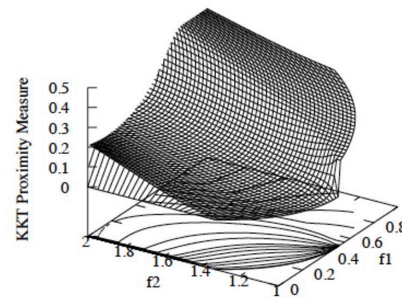
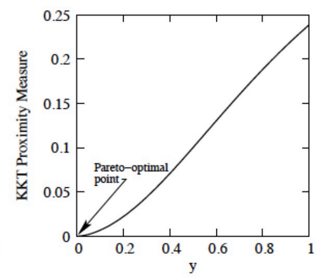
KKT Proximity Metric on P1

- Smooth reduction to zero





- Contour parallel to PO front

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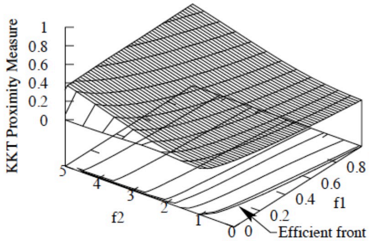
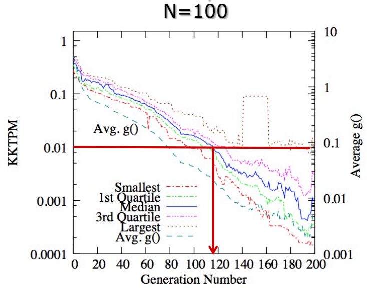
ZDT1 Test Problem with NSGA-II

KKTPM Surface



NSGA-II Populations N=100



- KKTPM parallel to PO front
- Population converges as a front

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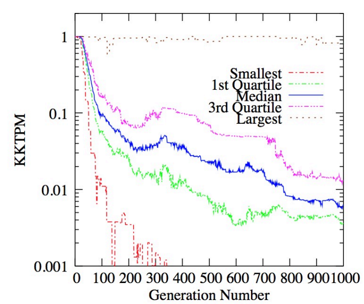
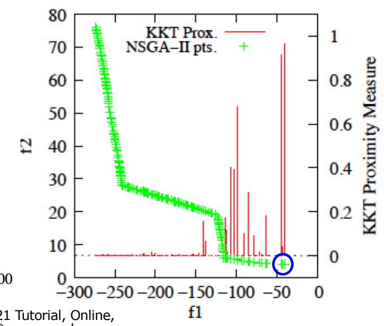
Problem OSY with NSGA-II

- 25% points did not converge until 250 gen.
- Local search to speed up EMO runs





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Progressively Interactive EMO (PI-EMO)

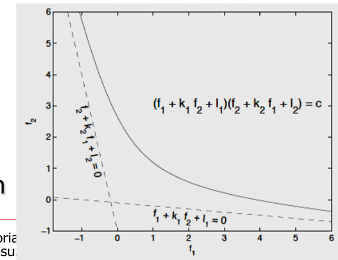
- Deb, Sinha, Korhonen and Wallenius, 2010 (IEEE TEC)
- Preference information during an EMO run
  - Ask DM after a few generations
  - Modify search thereafter
  - Continue till convergence
- Future of preference-based EMO
- Branke et al. (EMO-2009) and others

Utility Function

- Choose k well-distributed non-dominated points
- Ask DM for pair-wise information
- Form a utility function:

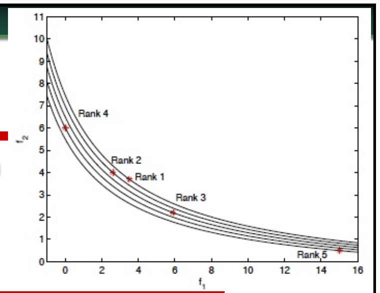
$$V(f_1, f_2) = (f_1 + k_1 f_2 + l_1)(f_2 + k_2 f_1 + l_2)$$

- Can be generalized to any number of objectives
- Parameters k_i, l_i are to determined by solving an optimization problem



Forming Utility Function

- Solve following problem with k_i, l_i, and ε as variables:

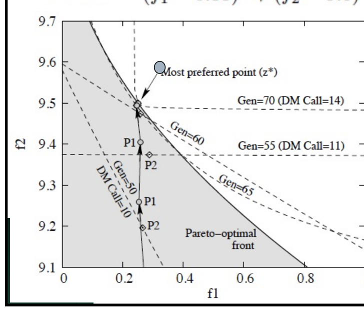


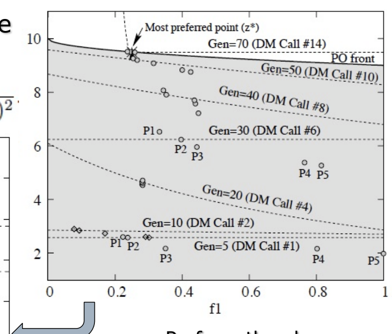
$$
\begin{array}{ll}
\text{Maximize} & \epsilon, \\
\text{subject to} & V \text{ is non-negative at every point } P_i, \\
& V \text{ is strictly increasing at every point } P_i, \\
& V(P_i) - V(P_j) \geq \epsilon, \quad \text{for all } (i,j) \text{ pairs} \\
& \qquad \text{satisfying } P_i \succ P_j, \\
& |V(P_i) - V(P_j)| \leq \delta_V, \quad \text{for all } (i,j) \text{ pairs} \\
& \qquad \text{satisfying } P_i \equiv P_j.
\end{array}
$$

PI-EMO Results

- ZDT1 with a preference function:

$$V(f_1, f_2) = \frac{1}{(f_1 - 0.35)^2 + (f_2 - 9.6)^2}.$$

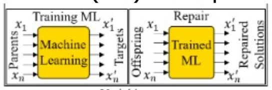


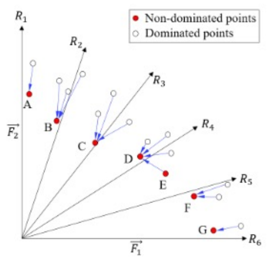


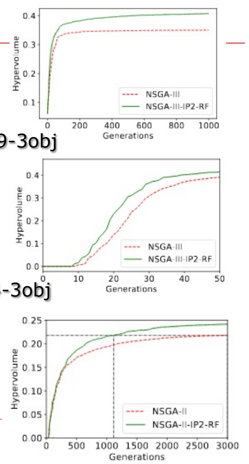
Perform the above with minimum number of DM calls

Machine Learning to Improve EMO's Performance

- Learn from EMO's progress
- Use ML (RF) to repair







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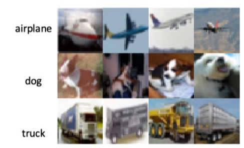
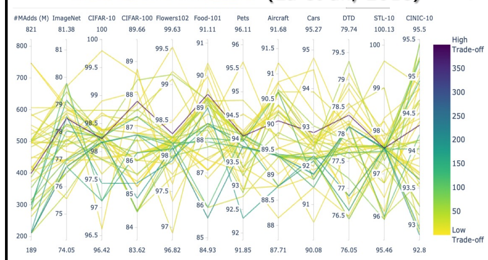
EMO in Machine Learning

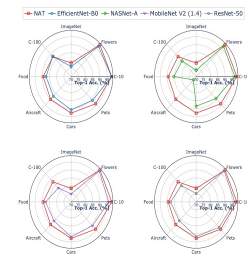
- Accuracy and Complexity by NSGANet for NAS



EMO finds better neural architecture than other methods (Lu et al., 2018)

- Transfer Learning based NAS
- Uses a Supernet for faster learning
- Many-obj NSGA-III to find NAS for 11 problems (Lu et al., 2020)





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Conclusions

pymoo Demonstration by Julian Blank is next

- EMO is a fast-growing field of research and application
  - Exciting field within GEC
- Practical applns. continuously addressed
- EMO+MCDM, EMO+Math optimization
- EMO is diversifying into new areas
- Commercial softwares available
  - Heeds, ModeFrontier, iSight, VisualDoc
- Computer codes freely downloadable
  - pymoo, Jmetal, PISA, MOEAFramework, EMOO websites
- Most downloaded EC papers are from EMO

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Goal

Julian Blank

Practical Introduction to Multi-objective Optimization (in Python) using pymoo

- **Part 1:** Define an exemplary constrained bi-objective optimization problem
- **Part 2:** Implement the problem in Python using pymoo and optimize it using NSGA-II
- **Part 3:** Analyze the obtained results
- **Part 4:** Some more useful information and features available in pymoo

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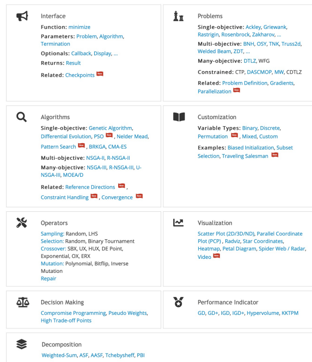
pymoo
Multi-objective Optimization in Python

- State of the art single- and multi-objective optimization algorithms
- Many more features related to multi-objective optimization such as visualization and decision making
- Python
- Founded in 2019
- Main Developer: Julian Blank
- Documentation available at https://pymoo.org
- **pip install pymoo==0.4.2.2**

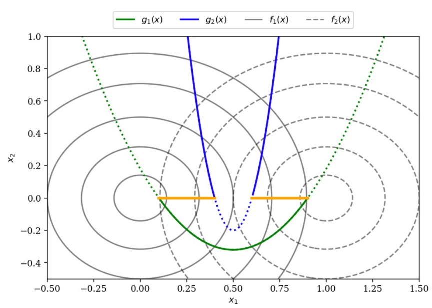


Walkthrough

1. Define Problem mathematically (and transform it)
2. Implement the Problem
3. Choose an Algorithm and Define its Hyper-parameters
4. Execute the Algorithm and Obtain Results
5. Analyze the Results including Visualization and Decision Making

1. Problem Definition
Constrained Bi-Objective Problem

$$\begin{aligned} \min \quad & f_1(x) = (x_1^2 + x_2^2) \\ \max \quad & f_2(x) = -(x_1 - 1)^2 - x_2^2 \\ \text{s.t.} \quad & g_1(x) = 2\,(x_1 - 0.1)\,(x_1 - 0.9) \le 0 \\ & g_2(x) = 20\,(x_1 - 0.4)\,(x_1 - 0.6) \ge 0 \\ & -2 \le x_1 \le 2 \\ & -2 \le x_2 \le 2 \end{aligned}$$



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$\longrightarrow$

$$\begin{aligned} \min \quad & f_1(x) = (x_1^2 + x_2^2) \\ \min \quad & f_2(x) = (x_1 - 1)^2 + x_2^2 \\ \text{s.t.} \quad & g_1(x) = 2\,(x_1 - 0.1)\,(x_1 - 0.9)\,/\,0.18 \le 0 \\ & g_2(x) = -20\,(x_1 - 0.4)\,(x_1 - 0.6)\,/\,4.8 \le 0 \\ & -2 \le x_1 \le 2 \\ & -2 \le x_2 \le 2 \end{aligned}$$

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2. Implement the Problem

- Inherit from the *Problem* class
  - Set the meta information such as number of variables, objectives, constraints
  - Implement the evaluation function *_evaluate*

```python
import autograd.numpy as anp
import numpy as np

from pymoo.model.problem import Problem


class CantileveredBeam(Problem):

    def __init__(self):
        super().__init__(n_var=4, n_obj=1, n_constr=2, type_var=np.double
        self.xl = np.array([2, 0.1, 0.1, 3.0])
        self.xu = np.array([12.0, 1.0, 2.0, 7.0])
        self.h1 = np.array([0.1, 0.25, 0.35, 0.5, 0.65, 0.75, 0.9, 1.0])

    def _evaluate(self, x, out, *args, **kwargs):
        E, L, P = 1e7, 36.0, 1000.0

        b1, h1, b2, H = x[:, 0], x[:, 1], x[:, 2], x[:, 3]
        I = 1 / 12 * b2 * (H - 2 * h1) ** 3 + 2 * (1 / 12 * b1 * h1 ** 3
        volume = (2 * h1 * b1 + (H - 2 * h1) * b2) * L
        out["F"] = volume

        sigma = P * L * H / (2 * I)
        delta = P * L ** 3 / (3 * E * I)

        g1 = (sigma - 5000.0) / 5000.0
        g2 = (delta - 0.1) / 0.1
        out["G"] = anp.column_stack([g1, g2])
```

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3. Choose an Algorithm and Define its Hyper-parameters

```python
from pymoo.algorithms.nsga2 import NSGA2
from pymoo.factory import get_sampling, get_crossover, get_mutation

algorithm = NSGA2(
    pop_size=40,
    n_offsprings=10,
    sampling=get_sampling("real_random"),
    crossover=get_crossover("real_sbx", prob=0.9, eta=15),
    mutation=get_mutation("real_pm", eta=20),
    eliminate_duplicates=True
)
```

Some modifications by varying the hyperparameters might require a deeper algorithm-specific understand

- The Algorithm choice is not always straightforward and often requires some experience in optimization
- Here, for a constrained bi-objective problem, NSGA-II is a reasonable choice

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4. Execute the Algorithm and Obtain Results

- Define a Termination Condition and run the algorithm
- Waiting until the algorithm has terminated and store the results in an object `res`

```python
from pymoo.factory import get_termination

termination = get_termination("n_gen", 40)

from pymoo.optimize import minimize

res = minimize(problem,
               algorithm,
               termination,
               seed=1,
               save_history=True,
               verbose=True)
```

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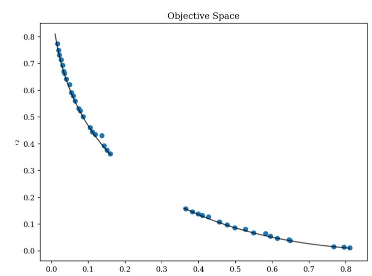
5. Analyze the Results including Visualization and Decision Making

- Analyze the obtained results
- Simple ways to make to a decision
- Support for different visualization techniques for more than 3 objectives.



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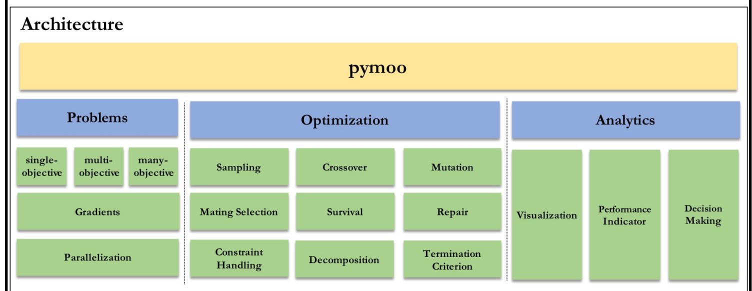
Live Demonstration

Architecture



Advanced Features

- Checkpointing
- Biased Initialization
- Callback
- Uniform Reference Directions

Final Words

- Work in Progress
- Contributions Welcome!

Thank you!