

Tutorial: Multi-Objective Optimization and Recommendations



Part 1: Multi-Objective Optimization

David Wang
Principal Data Scientist
Morningstar, Inc.

11/29/2022

Time: 10:30 - 12:00 ET



Contents

- Background and History
- Multi Objective Optimization (MOO) Basic
- MOO Algorithms
 - Scalarization Algorithms
 - Multi Objective Evolutionary Algorithms
 - Algorithm Evaluation Based on Pareto Set
- Selection of a Single Solution in Pareto Set
- MOO Libraries
- Summary & QA

Background

- Multi Objective Optimization Problems Everywhere

Consumer



Price ↓
Fuel consumption ↓
Comfort ↑
Performance ↑

Central Bank



Inflation ↓
Unemployment ↓
Trade deficit ↓

Engineer



Performance ↑
Cost ↓

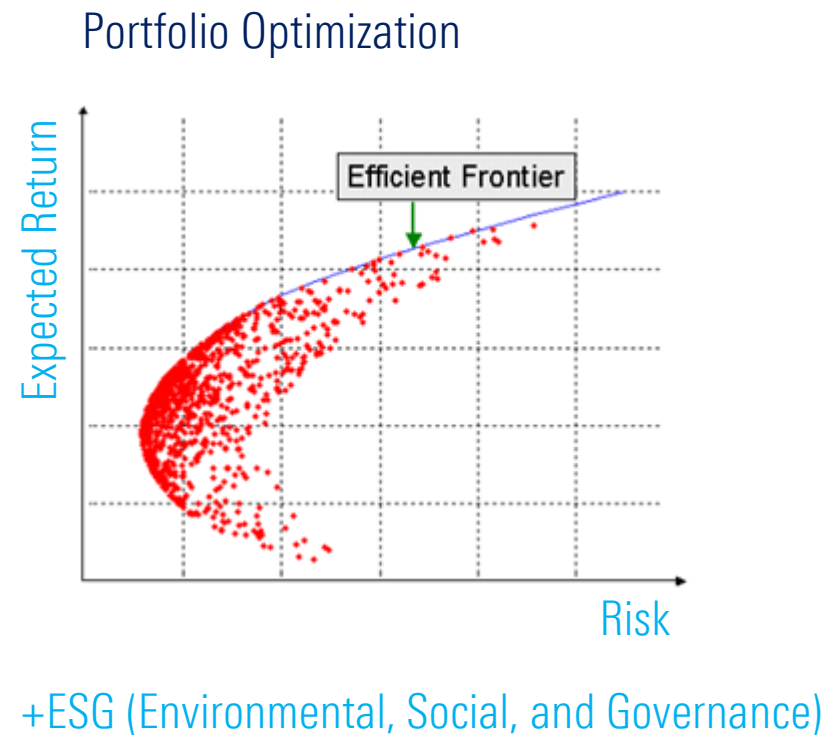
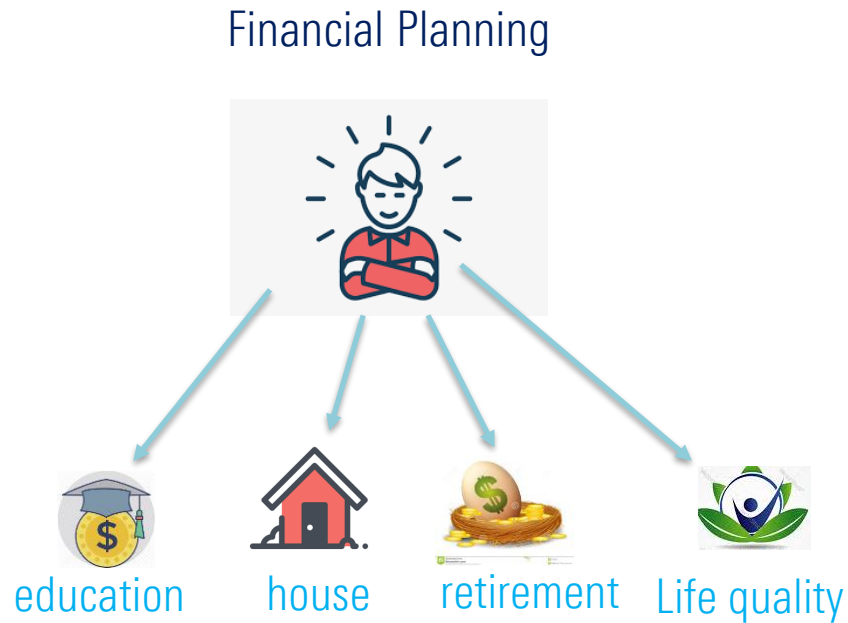
Communication



Data rate (bandwidth) ↑
Latency ↓
Energy consumption ↓

Background

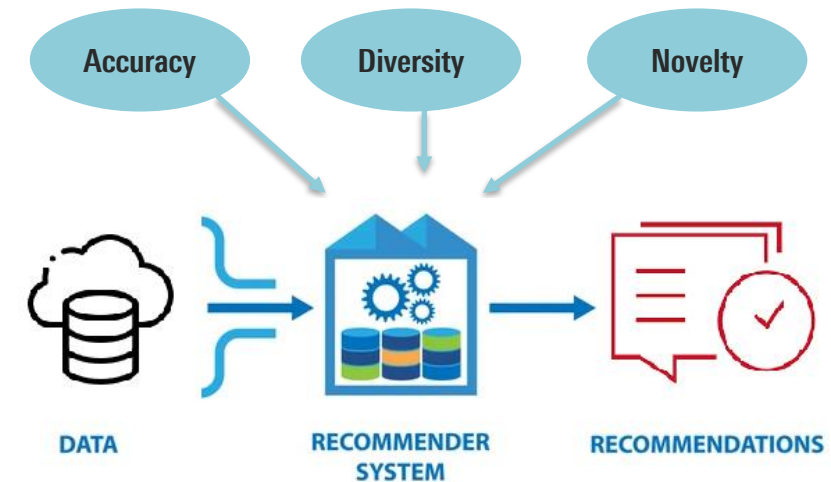
- Multi Objective Optimization in Finance



Background

■ Multi Metrics in Recommendation Systems

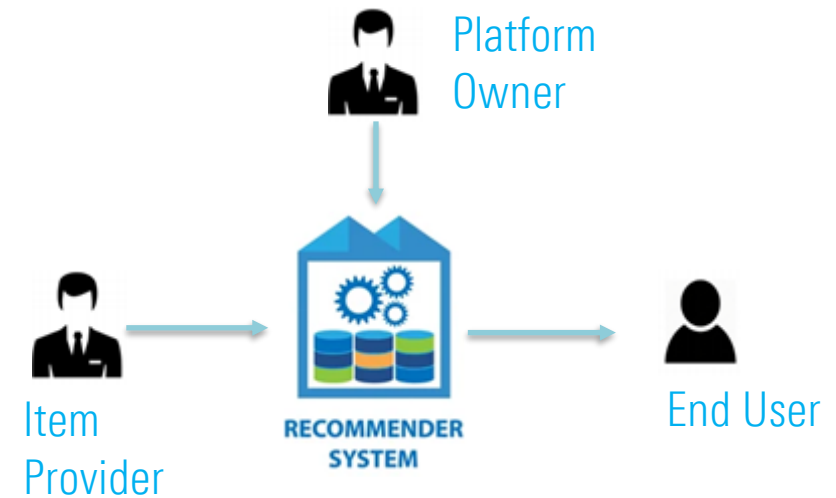
- Goal: Meets user's need
- Objectives:
 - Maximize Accuracy
 - Maximize Diversity
 - Maximize Novelty
- Challenge
 - Increase Diversity may decrease Accuracy
 - Increase Novelty may decrease Accuracy



Background

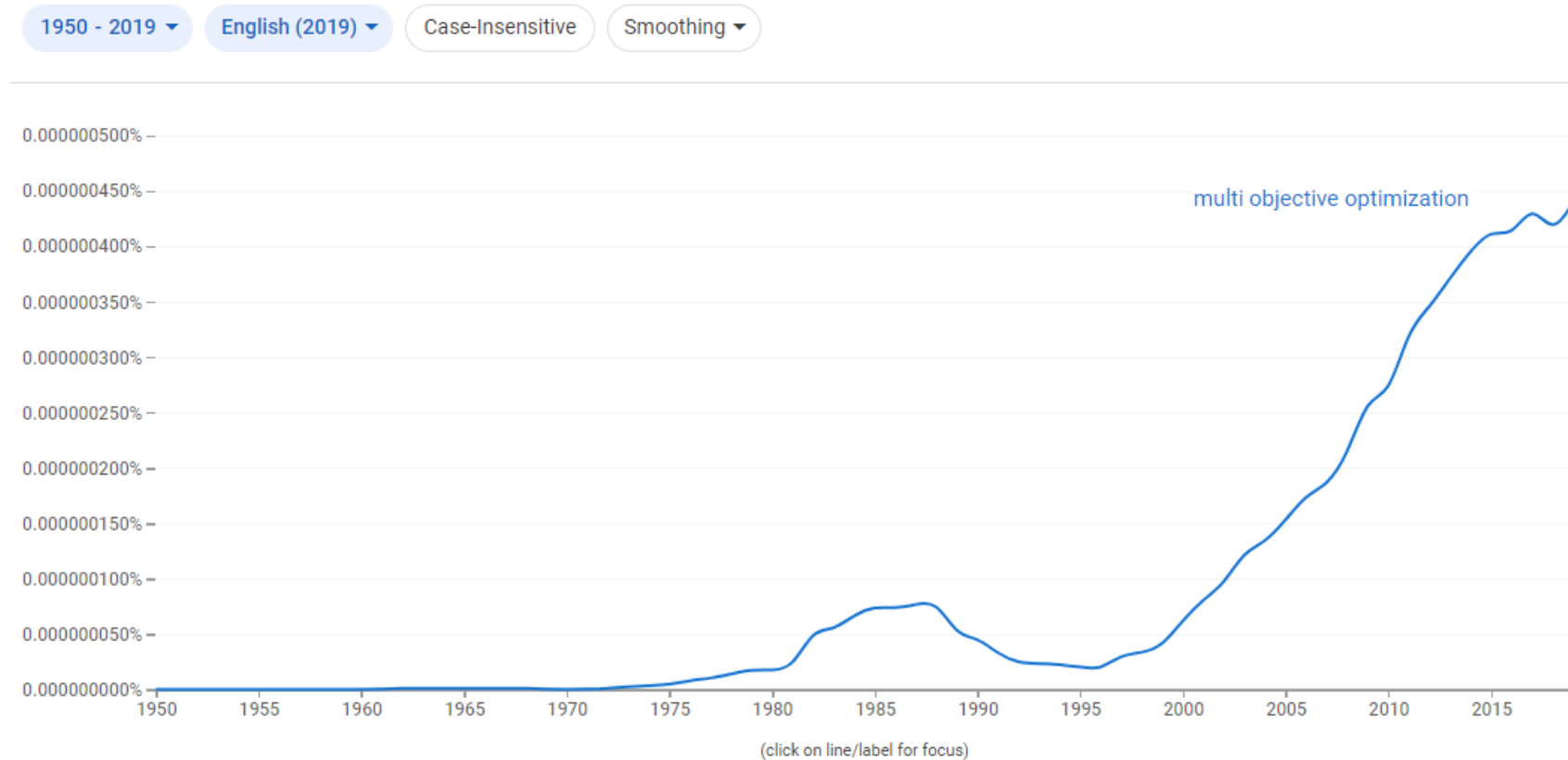
■ Multi Stakeholder Recommendation Systems

- Goal: Meet interests of **all stakeholders**
- Objectives: Maximize **Three Utilities**
 - In respect of **End User**
 - In respect of **Provider**
 - In respect of **Platform Owner**
- Challenge
 - Utilities regarding to three stakeholders may **conflict** each other



Background

■ MOO Research is Becoming Popular

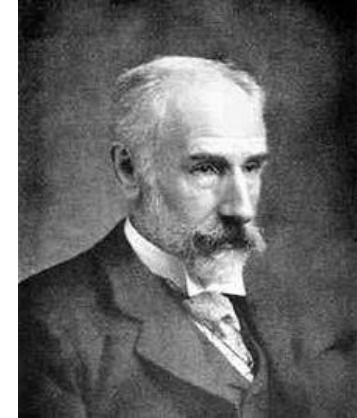


- Sources: https://books.google.com/ngrams/graph?content=multi+objective+optimization&year_start=1950&year_end=2019&corpus=26&smoothing=3

History

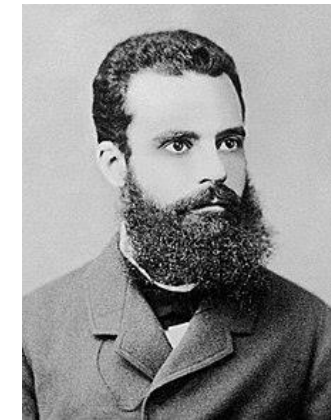
- Francis Ysidro Edgeworth (1845-1926)

- ***Mathematical Psychics: An Essay on the Application of Mathematics to the Moral Sciences***, published in 1881
- “It is required to find a point (x, y) such that, in whatever direction we take an infinitely small step, P and Π **do not increase together**, but that, while one increases, the other decreases”



- Vilfredo Pareto (1848-1923)

- ***Manual of Political Economy***, published in 1906
- Formally defined ‘**Pareto optimal**’
- “The **optimum** allocation of the resources of a society is not attained so long as it is possible to make at **least one individual better off** in his own estimation while keeping others as well off as before in their own estimation.”



Contents

- Background and History
- Multi Objective Optimization (MOO) Basic
- MOO Algorithms
 - Scalarization Algorithms
 - Multi Objective Evolutionary Algorithms
 - Algorithm Evaluation Based on Pareto Set
- Selection of a Single Solution in Pareto Set
- MOO Libraries
- Summary & QA

Multi Objective Optimization (MOO): Definition

- Multi Objective Optimization (MOO) Problem

$$\min_{\mathbf{x}} (f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_M(\mathbf{x}))$$

Subject to:

$$\begin{aligned} g_j(\mathbf{x}) &\geq 0, & j &= 1, 2, \dots, J \\ h_k(\mathbf{x}) &= 0, & k &= 1, 2, \dots, K \\ x_i^L &\leq x_i \leq x_i^U, & i &= 1, 2, \dots, n \end{aligned}$$

Decision variable: $\mathbf{x} \in \mathbf{R}^n$

Objective Functions: $f_i, i = 1, 2, \dots, M, (f_1, f_2, \dots, f_M) \in \mathbf{R}^M,$

Feasible Solutions: $S \subseteq \mathbf{R}^n$

$$S = \{x \mid x_i^L \leq x_i \leq x_i^U, g_j(x) \geq 0, h_k(x) = 0, j = 1, 2, \dots, J, k = 1, 2, \dots, K, i = 1, \dots, n\}$$

Multi Objective Optimization (MOO): Example

- Example: Two Objectives (metrics) in Recommender Systems

Name	Symbol	Meaning
Decision Variable	x	A Top N recommendation list
Feasible Solution Set	S	All top N recommendations
First Objective	$f_1(x)$	1 – accuracy
Second Objective	$f_2(x)$	1 – diversity

- Find recommendation list that maximize accuracy and diversity

$$\min_{x \in S} (f_1, f_2) \quad \text{or} \quad \min_{x \in S} F(x), \text{ where } F(x) = (f_1, f_2)$$

Multi Objective Optimization (MOO): Special Features

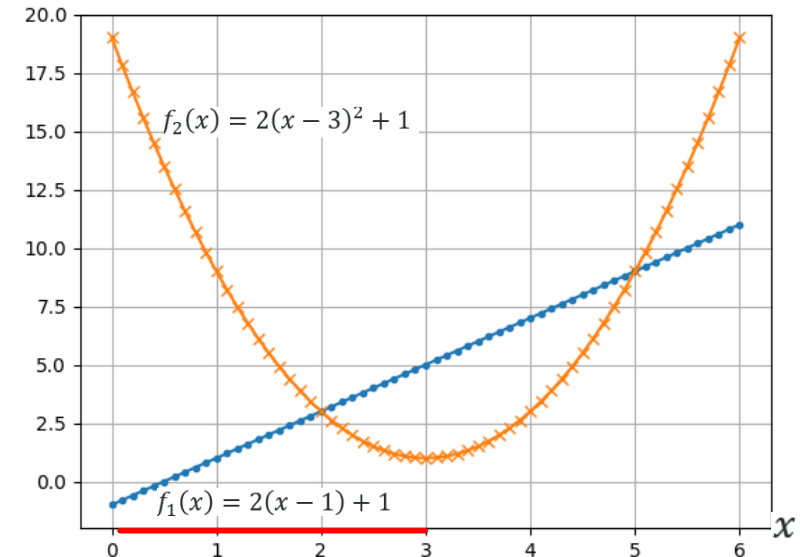
- Special Characteristic of MOO
 - Objectives may be conflict each other
 - Cannot determine which solution is better
 - Example:

$$\min_x (f_1, f_2)$$

$$\text{Where } f_1(x) = 2(x - 1) + 1,$$

$$f_2(x) = 2(x - 3)^2 + 1$$

$$\text{Subject } x \in [0, 6]$$



Multi Objective Optimization (MOO): Dominance Relation

■ Dominance Relation

A solution x is said to be **Dominated by** x^* if and only if

$$f_m(x^*) \leq f_m(x) \text{ for all } m = 1, 2, \dots, M$$

and there exists **at least one** m' such that:

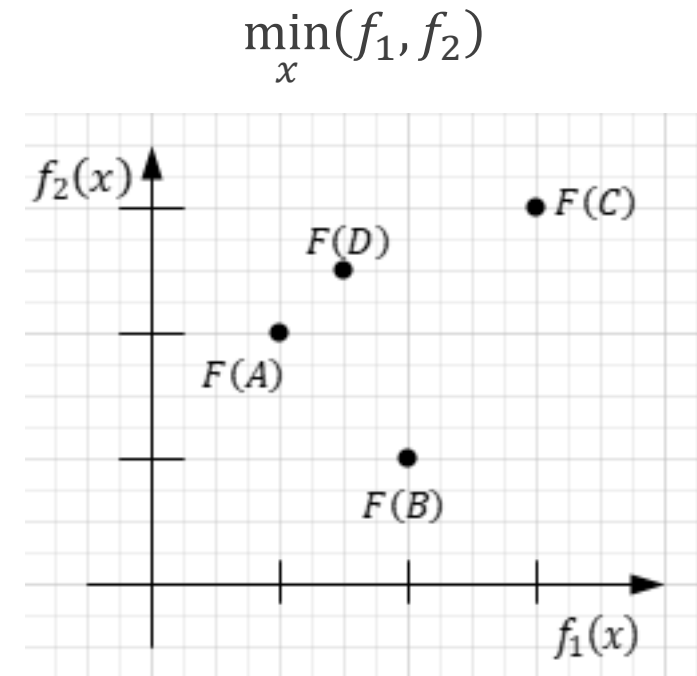
$$f_{m'}(x^*) < f_{m'}(x)$$

A and B **dominate** C,

D is only **dominated by** A.

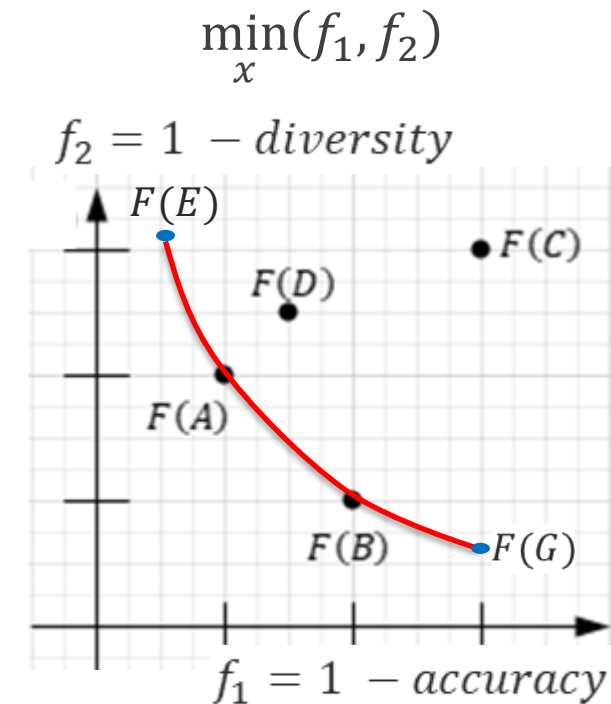
A and B: no dominance relationship

D and B: no dominance relationship



Multi Objective Optimization (MOO): Pareto Optimal

- **Non-Dominated Solution** (Pareto Optimal Solution)
 - Not dominated by any other solutions
 - Solution A , B , E and G are Pareto Optimal
- **Pareto Optimal Set** (in decision variable space):
 - All x such that $F(x)$ is on curve from $F(E)$ to $F(G)$
- **Pareto Front** (in objective space):
 - All $F(x)$ on curve from $F(E)$ to $F(G)$



Multi Objective Optimization (MOO): Example

- Example:

$$\min_x (f_1, f_2)$$

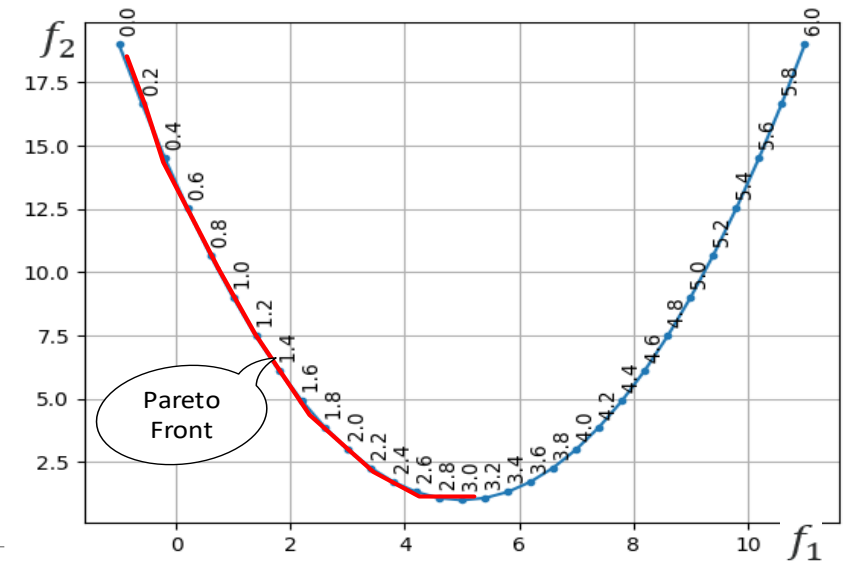
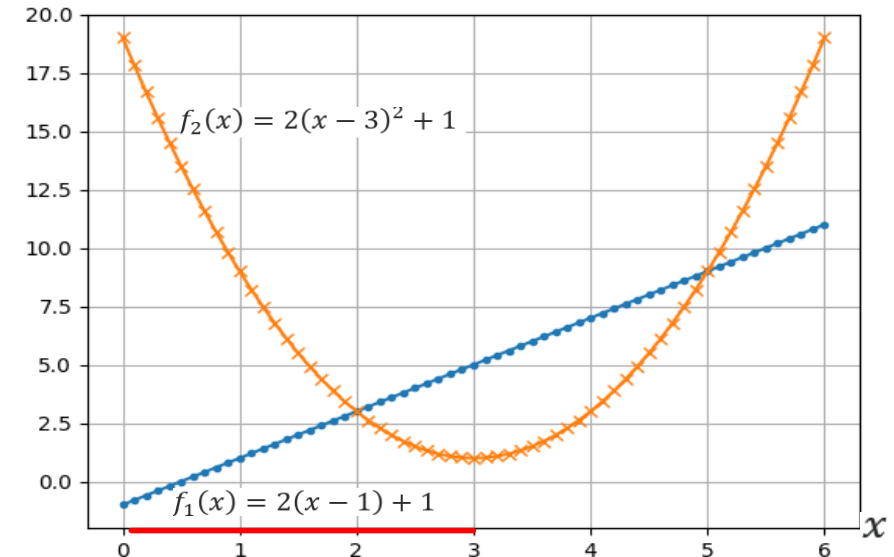
Where $f_1(x) = 2(x - 1) + 1$,

$$f_2(x) = 2(x - 3)^2 + 1$$

Subject $x \in [0, 6]$

- Analysis

- Feasible solutions: $S = [0, 6]$
- Pareto Set: $\{x \mid x \in [0, 3]\}$
- Pareto Front: $\{(f_1, f_2) \mid x \in [0, 3]\}$



Multi Objective Optimization (MOO): Goals

- Solving Multi Objective Optimization (MOO) Problem

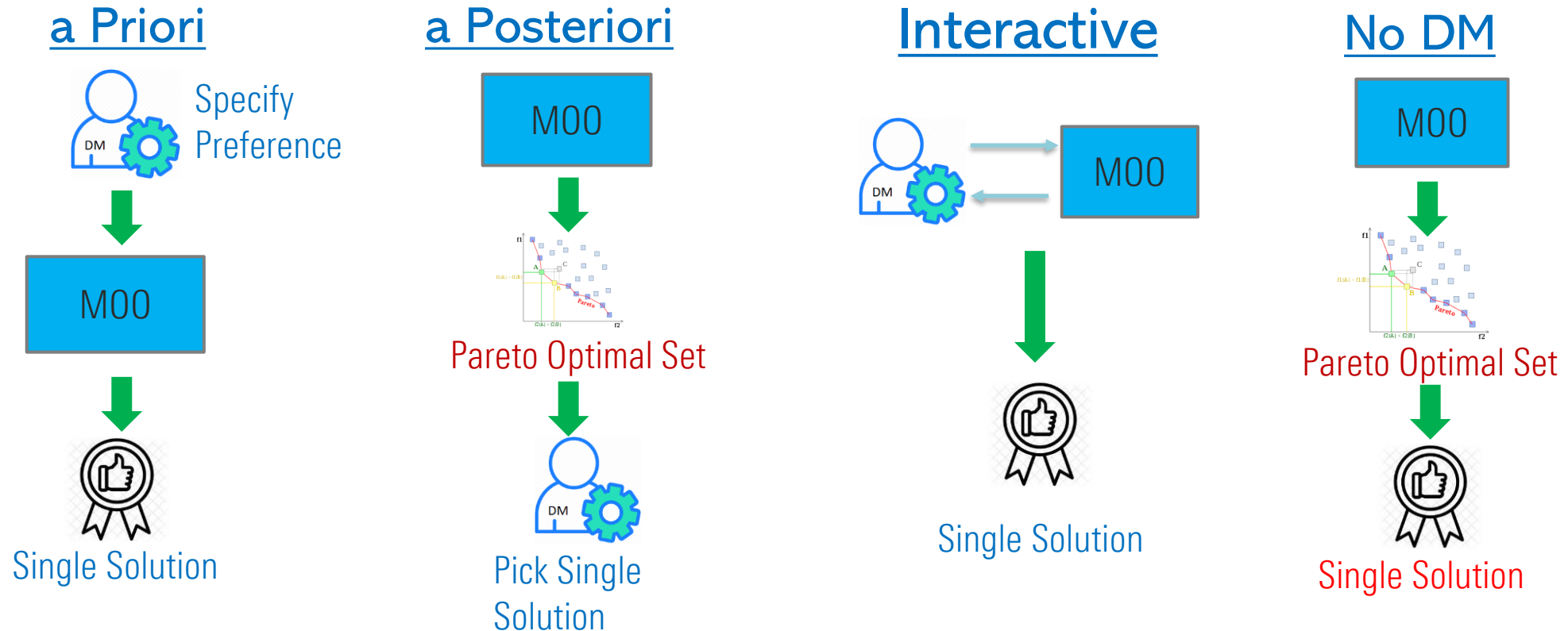
$$\min_{\mathbf{x} \in S} F(\mathbf{x})$$

where $F(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_M(\mathbf{x}))$
 $\mathbf{x} \in S$
 S is set of all feasible solutions

- Outputs
 - Find a Non-Dominated Solution
 - Find All Non-Dominated Solutions (Pareto Set)

Multi Objective Optimization (MOO): Decision Making Process

- MOO Decision Making Process



Multi Objective Optimization (MOO): Decision Making Process

- MOO Decision Making Process

DM Method	DM Preference Stage	Pareto Set Needed	Use Case
A Priori	Before	No	DM know the preference of objective
A Posteriori	After	Yes	DM not clear about objective preference
Interactive	Middle	No	DM know the objective preference
No DM	Not available	Yes	DM is not available

Multi Objective Optimization (MOO): Algorithms Summary

■ Scalarization Algorithms

- Transform multi-objectives into a single objective
- Solve it by single objective optimizer
- Find one Pareto optimal solution in one run
- Find Pareto Set in multiple run

■ Multi Objective Evolutionary Algorithms (MOEA)

- Follow natural evolution process such as gene evolution, a flock of birds seeking food and other resources, a cooling process of melted crystal, ...
- Find multiple Pareto optimal solutions in one run

Contents

- Background and History
- Multi Objective Optimization (MOO)
- MOO Algorithms
 - [Scalarization Algorithms](#)
 - Multi Objective Evolutionary Algorithms
 - Algorithm Evaluation Based on Pareto Set
- Selection of a Single Solution in Pareto Set
- MOO Libraries
- Summary & QA

Scalarization Algorithms

- Weighting Methods
- ϵ -Constraint Method
- Normal Boundary Intersection (NBI) & Normal Constraint (NC)
- Goal Programming
- Physical Programming
- Lexicographic Method

Scalarization Algorithms: Weighted Sum Methods

- Weighted Sum Method

- A weight vector based on DM preference of each objectives:

$$\min_x \sum_{i=1}^M w_i f_i(x)$$

subject to $x \in S$

Where $\sum_{i=1}^M w_i = 1$ and $w_i > 0$

- The condition of the weights guarantees Pareto optimal

Scalarization Algorithms: Weighted Sum Methods

- Example: Two Objective Metrics Recommender Systems

$$\min_{x \in S} (f_1, f_2), \quad f_1 = 1 - \text{accuracy}, f_2 = 1 - \text{diversity}$$

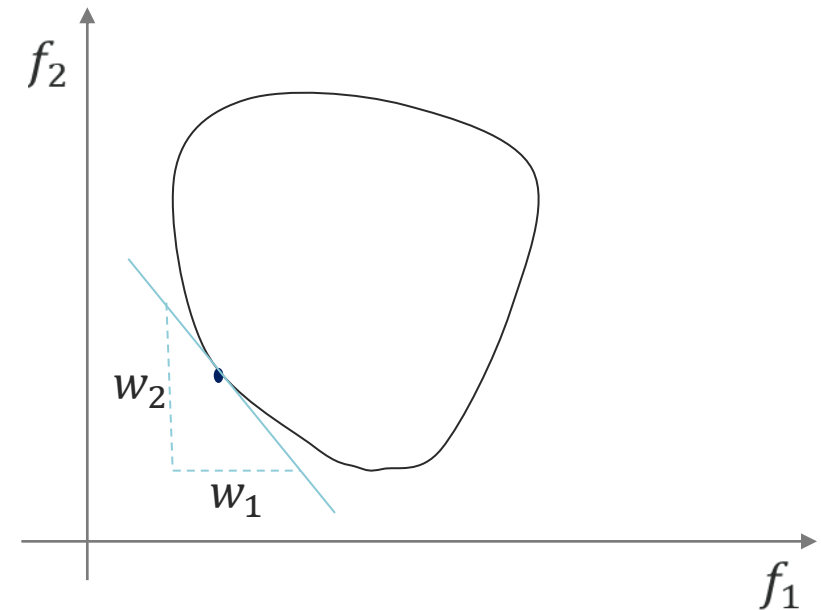
Solve: $\min_{x \in S} (w_1 f_1 + w_2 f_2)$

$$w_1 + w_2 = 1, w_1, w_2 > 0$$

- Each (w_1, w_2) gives one Pareto solution
- Question: Can we get **all** Pareto solutions in this way?

Scalarization Algorithms: Weighted Sum Methods

- **Question:** Can we get **all** Pareto solutions in this way?
 - Try all (w_1, w_2) ?
- **Answer:**
 - Not guaranteed
- **A Sufficient Condition¹**
 - **S is convex** in R^n
 - **Each objective function $f_k(x)$ is convex**



1. Yair Censor, *Pareto Optimality in Multiobjective Problems*, Applied Mathematics and Optimization 4, 41- 59

Scalarization Algorithms: Weighted Sum Methods

- A nonconvex problem(<https://commons.wikimedia.org/wiki/File:NonConvex.gif>)

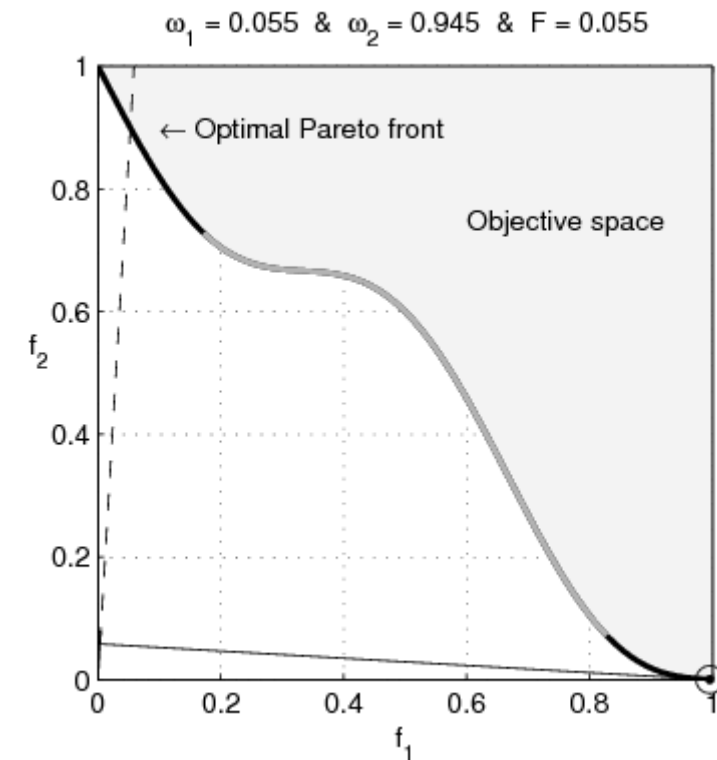
$$\min_x F(x) = w_1 f_1(x) + w_2 f_2(x)$$

Where $f_1(x) = x_1$

$$f_2(x) = 1 + x_2^2 - x_1 - 0.1\sin(3\pi x_1)$$

$$0 \leq x_1 \leq 1 \text{ and } -2 \leq x_2 \leq 2$$

Here f_2 is not convex on S



Scalarization Algorithms: Other Weighting Methods

- Weighted Exponential Sum¹

$$U = \sum_{i=1}^M w_i [f_i(x)]^p, f_i(x) > 0 \text{ for all } i = 1, 2, \dots, M$$

where $1 \leq p < \infty$, $\sum_{i=1}^M w_i = 1$ and $w_i > 0$

- 1) The condition of the weights guarantees the solution is Pareto optimal¹
- 2) Bigger p increase the effectiveness of finding all Pareto solutions

1. P. L. Yu, *A Class of Solutions for Group Decision Problems*, Management Science, Vol. 19, No. 8, Application Series (Apr., 1973), pp. 936-946

Scalarization Algorithms: Other Weighting Methods

- Weighted Metric Methods¹

$$U = \left[\sum_{i=1}^M w_i^p |f_i(x) - f_i^*|^p \right]^{\frac{1}{p}}$$

where $1 \leq p < \infty$, $\sum_{i=1}^M w_i = 1$ and $w_i > 0$

$f^* = (f_1^*, f_2^*, \dots, f_M^*)$ is ideal point in objective space

- 1) f^* : Utopian point (min value of each objective), goal point (specified by DM) or 0
- 2) The condition of the weights guarantees the solution is Pareto optimal
- 3) Bigger p increase the effectiveness of finding all Pareto solutions

1. P. L. Yu and G. Leitmann, *Compromise Solutions, Domination Structures, and Salukvadze's Solution*, Journal of Optimization Theory and Applications: Vol. 13, No. 3, 1974

Scalarization Algorithms: Other Weighting Methods

- Weighted Chebyshev method¹

$$U = \max_i \{w_i |f_i(x) - f_i^*|\}$$

where $\sum_{i=1}^M w_i = 1$ and $w_i > 0$

1) Taking $p \rightarrow \infty$ in $[\sum_{i=1}^M w_i^p |f_i(x) - f_i^*|^p]^{\frac{1}{p}}$

2) Can get complete Pareto set by changing weights without convex conditions²

3) May get non-Pareto solutions

1. Michael R. Lightner and Stephen W. Director, *Multiple Criterion Optimization for the Design of Electronic Circuits*, IEEE Transactions on Circuits and Systems, Vol. Cas-28, No. 3, March 1981
2. A. Messac and others. *Ability of Objective Functions to Generate Points on Nonconvex Pareto Frontiers*, AIAA JOURNAL, Vol. 38, No. 6, June 2000

Scalarization Algorithms: Other Weighting Methods

- Exponential Weighted Criterion¹

$$U = \sum_{i=1}^K (e^{p w_i} - 1) e^{p f_i(x)}, p \geq 1$$

Can find Pareto set in non-convex problem

- Weighted Product Method²

$$U = \prod_{i=1}^K |f_i(x)|^{w_i}$$

Minimize impact of different magnitude of objective function

1. Timothy Ward Athan & Panos Y. Papalambros, *A Note on Weighted Criteria Methods for Compromise Solutions in Multi-Objective Optimization*, Engineering Optimization, 27:2, 155-176
2. E. N. Gerasimov and V. N. Repko, *Multicriterial Optimization*, 1979, Plenum Publishing Corporation

Scalarization Algorithms: Weighting Methods Summary

Method	Formula	Pro	Con
Weighted Sum	$\sum_{i=1}^M w_i f_i(x)$	Simple	Require convex condition for Pareto set
Weighted Exponential Sums	$\sum_{i=1}^M w_i [f_i(x)]^p$	Increase p to approximate Pareto set	Bigger p may give non-Pareto solution
Weighted Metric Methods	$[\sum_{i=1}^M w_i^p f_i(x) - f_i^* ^p]^{\frac{1}{p}}$	Different choice of ideal points	Bigger p may give non-Pareto solution
Weighted Chebyshev method	$\max_i \{w_i f_i(x) - f_i^* \}$	Can find complete Pareto set	Some solution may not Pareto optimal
Exponential Weighted Criterion	$\sum_{i=1}^K (e^{pw_i} - 1)e^{pf_i(x)}$	Can find complete Pareto set	May lead computation overflow
Weighted Product Method	$\prod_{i=1}^K f_i(x) ^{w_i}$	Deal with different magnitude of objectives	Rarely used

Scalarization Algorithms: ϵ -Constraint

- ϵ -Constraint Method¹

$$\begin{aligned} & \min f_l(x) \\ & \text{subject to } f_i(x) \leq \epsilon_i, \text{ for all } i \neq l \\ & \epsilon_i \text{ is a known upper bound of } f_i \end{aligned}$$

- 1) Choose different ϵ_i may produce all Pareto solutions
- 2) No convex requirement
- 3) May not Pareto optimal

1. Haimes, Lasdon, Wismer, *On a Bicriterion Formulation of the Problems of Integrated, System Identification and System Optimization*, IEEE Transactions on Systems, Man, And Cybernetics, July 1971

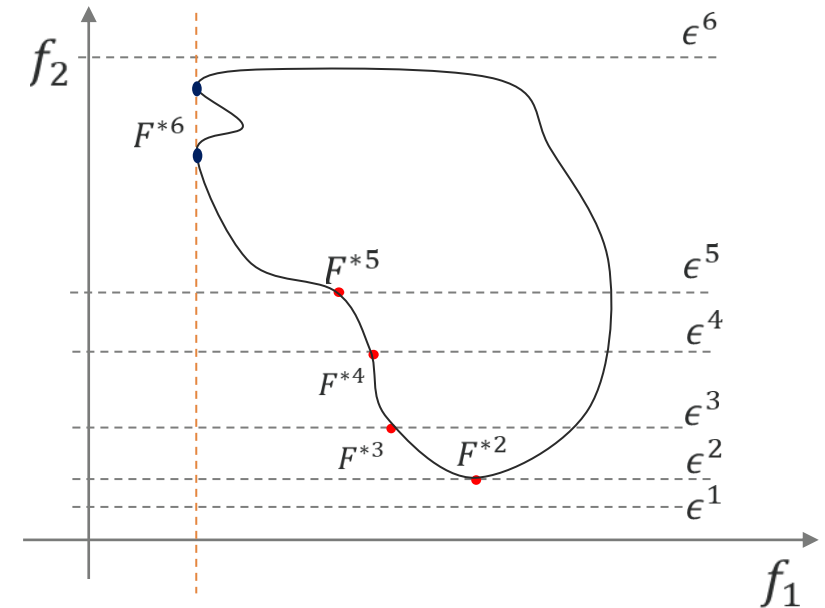
Scalarization Algorithms: ϵ -Constraint – a sufficient condition

- A sufficient condition of Pareto optimal¹
 - If optimal solution x^* is **unique**
- Two objective example

solve

$$\begin{array}{ll} \min_{x \in S} f_1(x) \\ \text{subject to } f_2 \leq \epsilon \end{array}$$

Constraint	Unique Solution	Pareto Optimal
ϵ^1	No solution	NA
$\epsilon^2, \epsilon^3, \epsilon^4, \epsilon^5$	Yes	Yes
ϵ^6	No	Not necessary



1. V. Chankong, Y. Haimes, Multiobjective Decision Making, Dover Publication, 1983

Scalarization Algorithms: NBI and NC

- Normal Boundary Intersection (NBI¹) and Normal Constraint (NC²)
 - Step 1: Find **Anchor Points** in objective space
 - Step 2: Define **Utopia Line(hyperplane)** connecting Anchor Points
 - Step 3: Set **evenly distributed** base points on Utopia Line
 - Step 4: Find Utopia line **normal vector** at each based point
 - Step 5: Optimize **one objective** in area **above normal vectors** at each base point

1. Das, Dennis, 1998: *Normal-boundary intersection: a new method for generating the Pareto surface in nonlinear multicriteria optimization problems*. SIAM J. Optim. 8, 631–657
2. Messac, Ismail-Yahaya, Mattson, 2003: *The normalized normal constraint method for generating the Pareto frontier*, Struct Multidisc Optim 25, 86–98 (2003)

Scalarization Algorithms : NBI & NC Method

- Example of two objective MOO problem

$$\min_x F(x), F(x) = (f_1, f_2)$$

- Anchor Points: A_1 and A_2

- A_1 : x^{*1} only minimize f_1

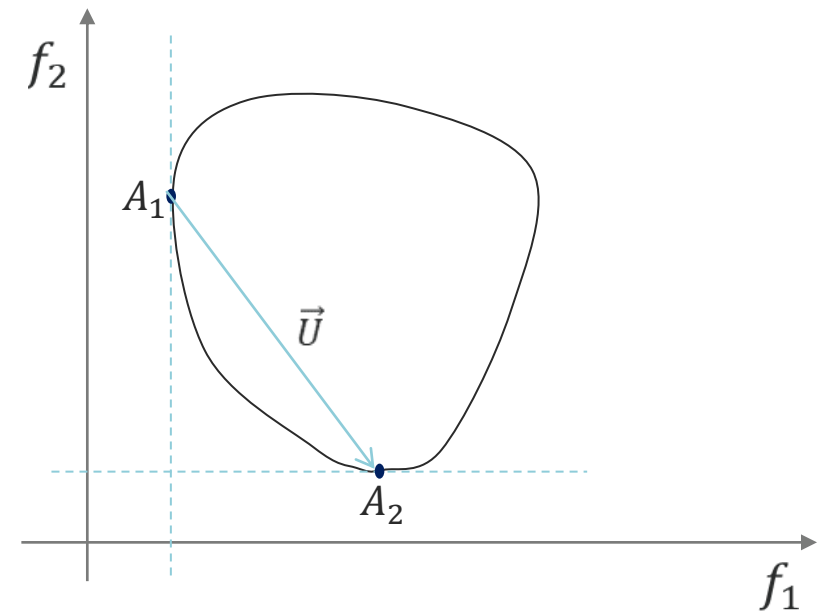
$$A_1 = (f_1^*(x^{*1}), f_2(x^{*1}))$$

- A_2 : x^{*2} only minimize f_2

$$A_2 = (f_1(x^{*2}), f_2^*(x^{*2}))$$

- Utopia Line Vector: $\overline{A_1 A_2}$:

$$\vec{U} = A_2 - A_1$$



Scalarization Algorithms: NBI & NC Method

- Set evenly distributed base points (F_{pj}) on Utopia Line (\vec{U})

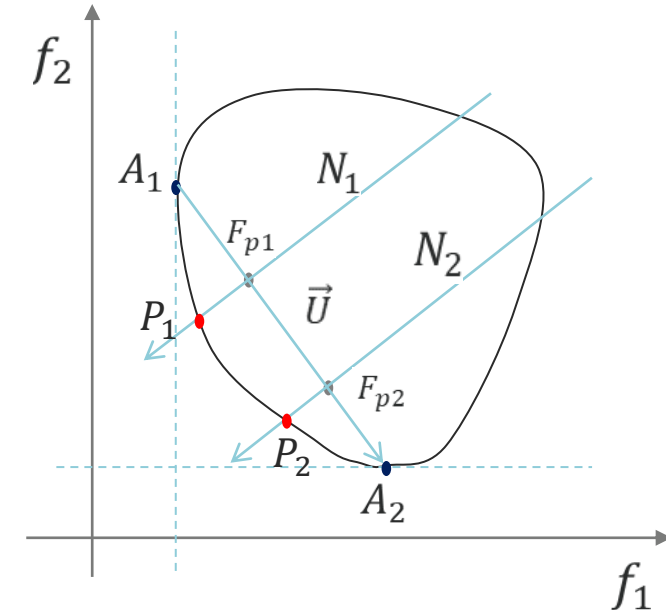
$$F_{pj} = \omega_{1j}A_1 + \omega_{2j}A_2$$

- Normal vector: \vec{N}_1, \vec{N}_2
- Optimize f_2 with new constraint

$$\min_x f_2(x)$$

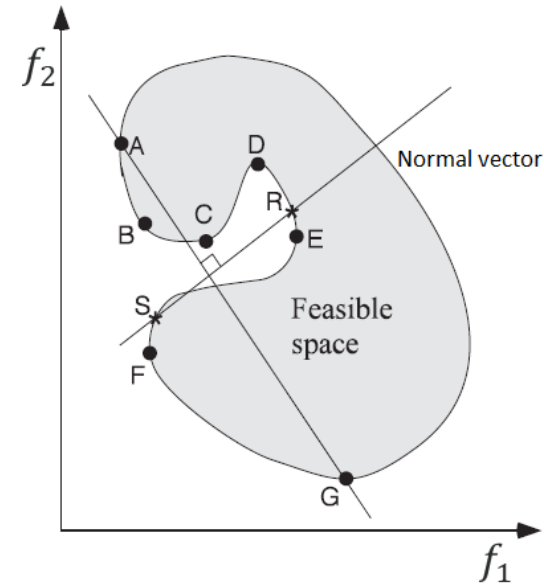
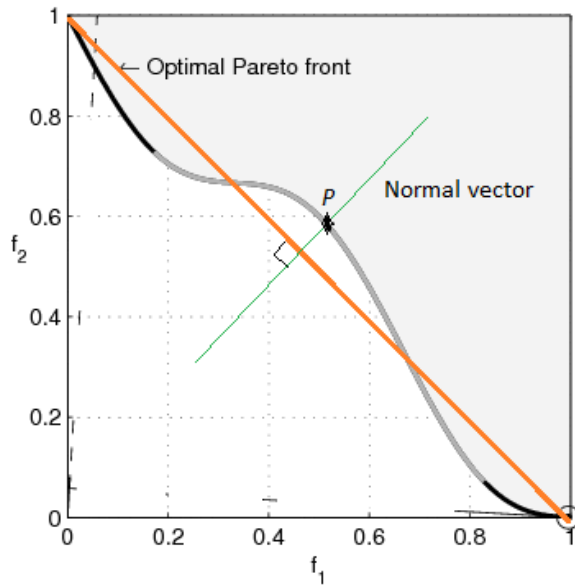
$$\text{subject to } \vec{U} \cdot (F(x) - F_{pj}) \leq 0,$$

- Pareto Optimal: P_1, P_2



Scalarization Algorithms: NBI & NC Method

- Works for non-convex case, may find Non-Pareto points: R



- Need to use filter to remove dominated points

Scalarization Algorithms: Other Methods

■ Other Scalarization Methods

Method	Idea	Scalarization	Characteristic
Goal Programming ¹	Set up goal for each objective	$\min \sum_{i=1}^M d_i $	May not be Pareto optimal
Physical Programming ²	Map goals and objective to utility functions \bar{g}_i	$\min \log_{10} \sum \bar{g}_i$	Pareto optimal Need detail knowledge of each objective
Lexicographic Method ³	Order each objective by importance	Minimize each objective in order	The solution may not be feasible

1. A. Charnes and W.W. Cooper, *Goal programming and multipleobjective optimizations*, European Journal of Operational Research I (1977) 39-54
2. Achille Messac, *Physical Programming: Effective Optimization for Computational Design*, AIAA JOURNAL Vol. 34, No. 1, January 1996
3. Peter C. Fishburn, *Exceptional Paper—Lexicographic Orders, Utilities and Decision Rules: A Survey*. Management Science 20(11):1442-1471 (1974)

Scalarization Algorithms: Summary

- Major scalarization methods summary

Method	be a Pareto Solution	To Get All Pareto Solutions	Other
Weighting methods	$\sum_{i=1}^M w_i = 1$ and $w_i > 0$	Convex for weighed sum	Some methods may get non-Pareto solution
ϵ -Constraint	Solution is unique	Solution is unique	May not get solution
Normal Bonded Intersection & Constraint	Pareto front is Convex	Pareto front is Convex	May get non-Pareto solution in concave case
Goal Programming	No guarantee	Not available	
Physical Programming	Guaranteed	Guaranteed	
Lexicographic Method	Not available	Not available	

Contents

- Background and History
- Multi Objective Optimization (MOO) Basic
- MOO Algorithms
 - Scalarization Algorithms
 - Multi Objective Evolutionary Algorithms
 - Algorithm Evaluation Based on Pareto Set
- Selection of a Single Solution in Pareto Set
- MOO Libraries
- Summary & QA

Multi Objective Evolutionary Algorithms

- Evolutionary Algorithms inspired by [natural evolutionary](#) process:

Genetic
Algorithm
(GA)



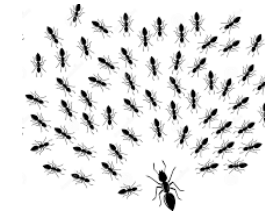
Particle Swam
Optimization
(PSO)



Simulated
Annealing
(SA)



Ant Colony
Optimal
(ACO)



Multi Objective Evolutionary Algorithms

- Benefits:

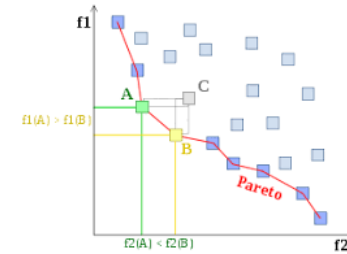


$f(x)$

Objective can
be any
function



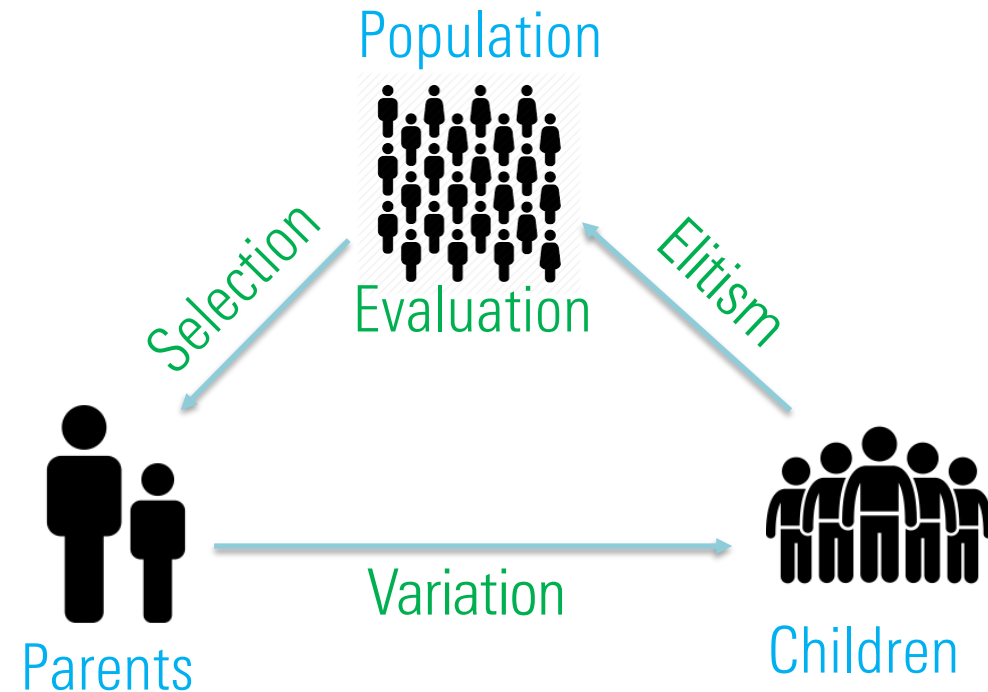
Parallel
computing



Get Pareto Set
in one run

Evolutionary Algorithms : Basic Concepts

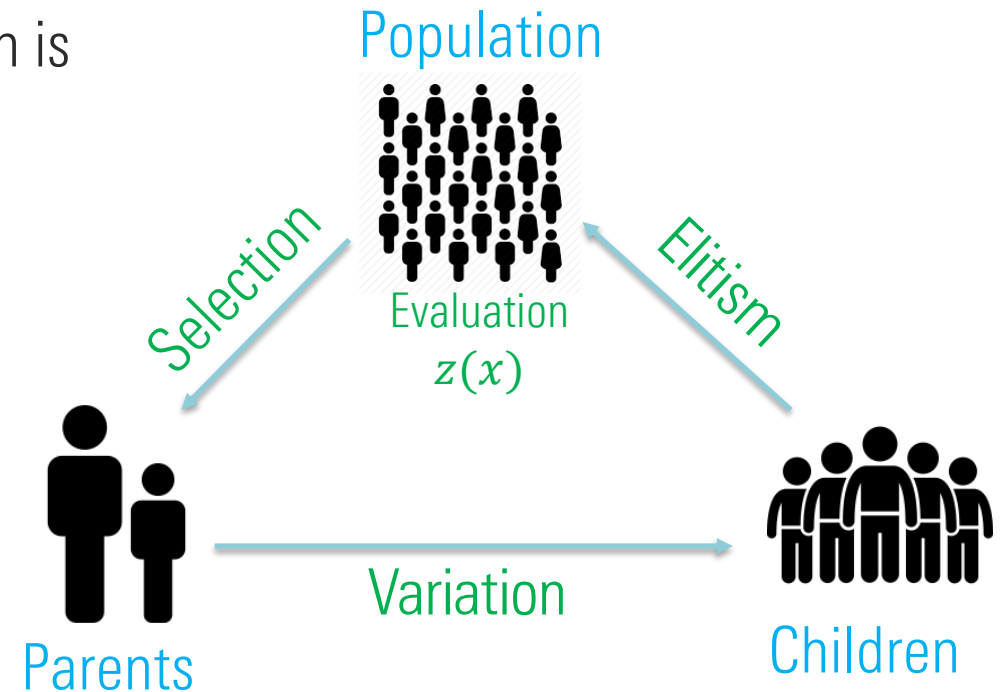
- Terminologies of Solutions:
 - **Individual** : a feasible solution x
 - **Population**: a set of individuals
 - **Parents**: selected from Population
 - **Children**: produced from Parents



Evolutionary Algorithms : Basic Concepts

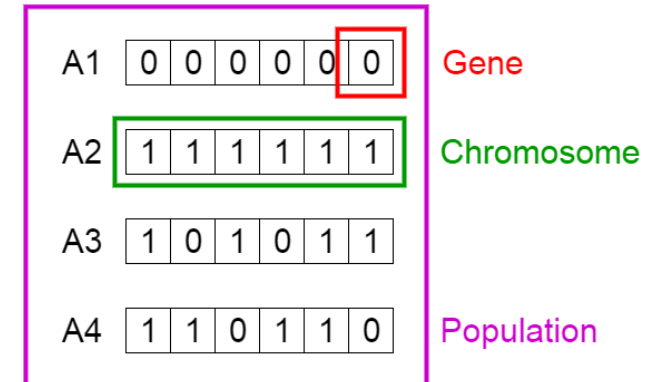
■ Operators of Genetic Algorithm

- **Evaluation**: measure how 'good' each solution is
 - assigning **fitness value (or order)**: $z(x)$
- **Selection**: find Parents
 - Random process
 - Tournament process
- **Variation**: produce children
 - Crossover
 - Mutation
- **Elitism**:
 - maintain '**better**' solution in each iteration



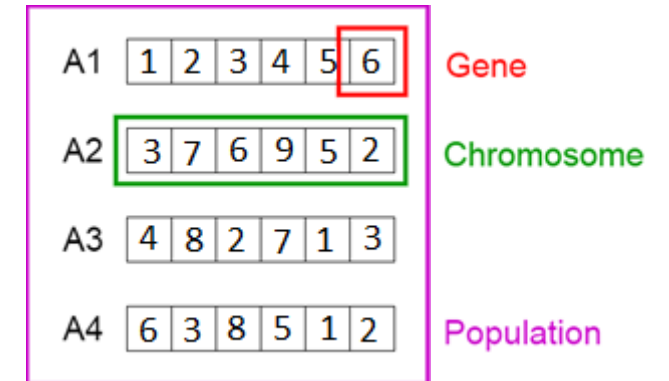
Evolutionary Algorithms : Encoding in Genetic Algorithm for RS

- Binary Encoding in Recommender System
 - Chromosome: a recommendation list (decision variable x)
 - Length of Chromosome = total number of available items
 - Each Gene position is corresponding an item
 - 1: item is in recommender list ,
 - 0: item is not in recommender list



Evolutionary Algorithms : Encoding in Genetic Algorithm for RS

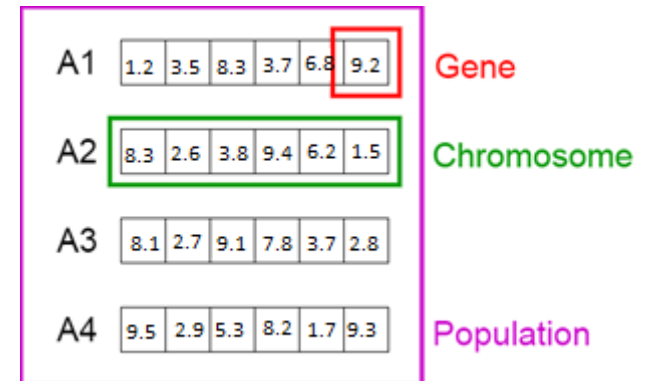
- **Permutation Encoding** in Recommender System
 - Length of **Chromosome** = N in top N recommendation list
 - The value of each **Gene**: **index** of an item
 - 6: the 6th item
 - Total 9 available items
 - $N = 6$



Evolutionary Algorithms : Encoding in Genetic Algorithm for parameters

■ Real Value Encoding for parameters

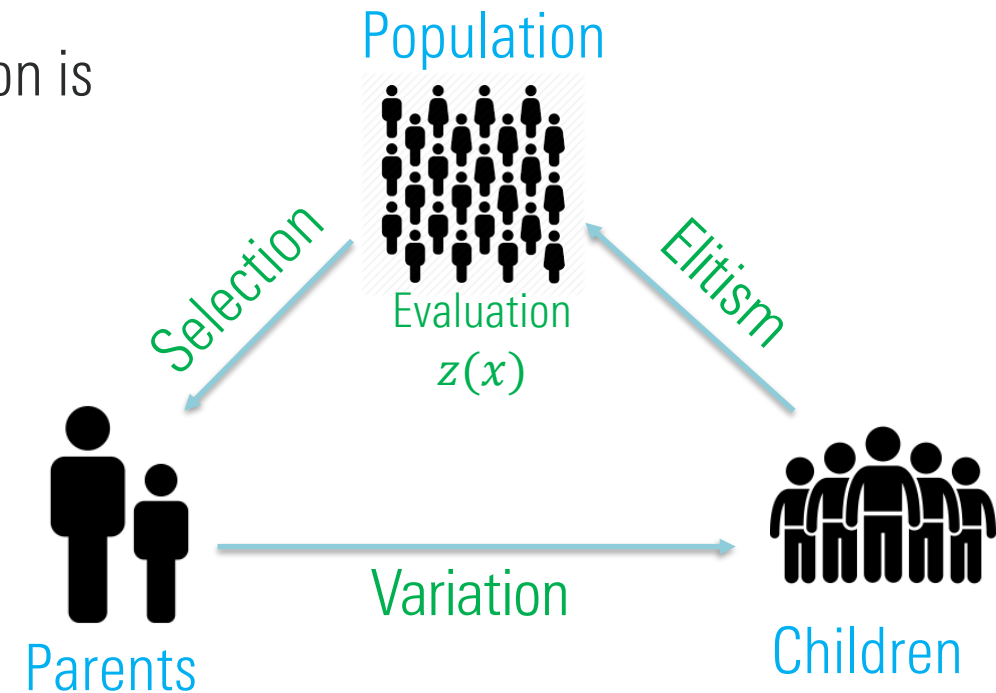
- **Chromosome**: a set of parameters (such as weights)
- Length of Chromosome = Number of parameters to be optimized
- Value in the **Gene**: value of the parameter
 - 6 parameters here
 - Parameter value is real value in $[1, 10]$



Summary: Single Objective Evolutionary Algorithms

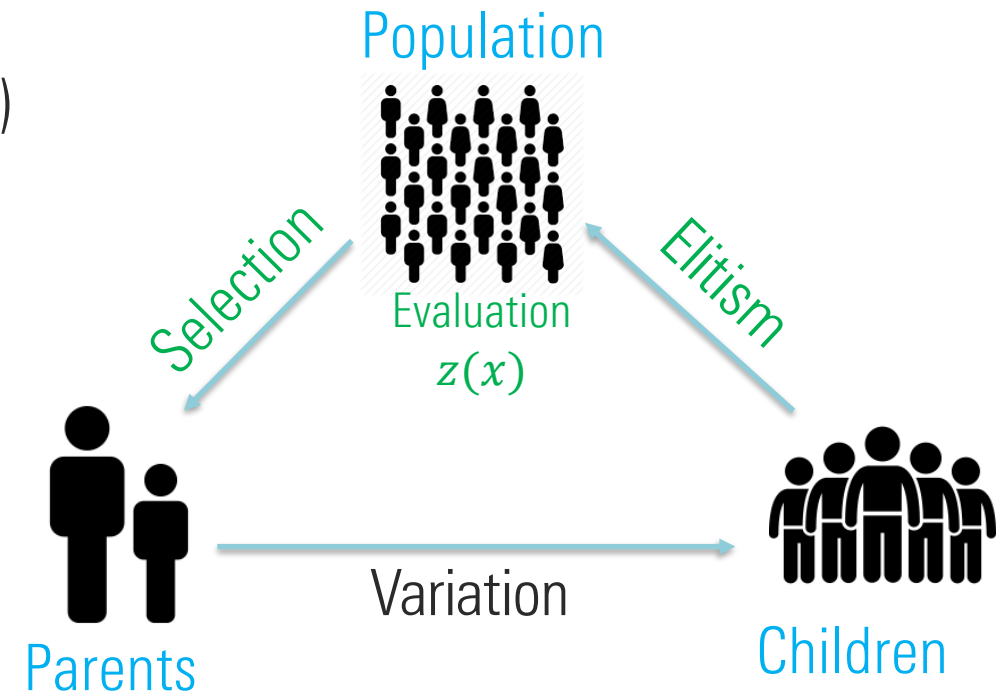
■ Operators

- **Evaluation:** measure how 'good' each solution is
 - assigning **fitness value (or order): $z(x)$**
- **Selection:** find Parents
 - Random process
 - Tournament process
- **Variation:** produce children
 - Crossover
 - Mutation
- **Elitism:**
 - maintain '**better**' solution in each iteration



From Single Objective to Multi Objective Evolutionary Algorithms

- Solve a MOO problem
 - Find non-dominated solutions (Pareto optimal)
- Where are multi objective considered?
Where are dominance relations applied?
 - Fitness value $z(x)$ evaluation
 - Parent selection
 - Elitism



Multi Objective Evolutionary Algorithms:

- Major MOO Genetic Algorithm Methods

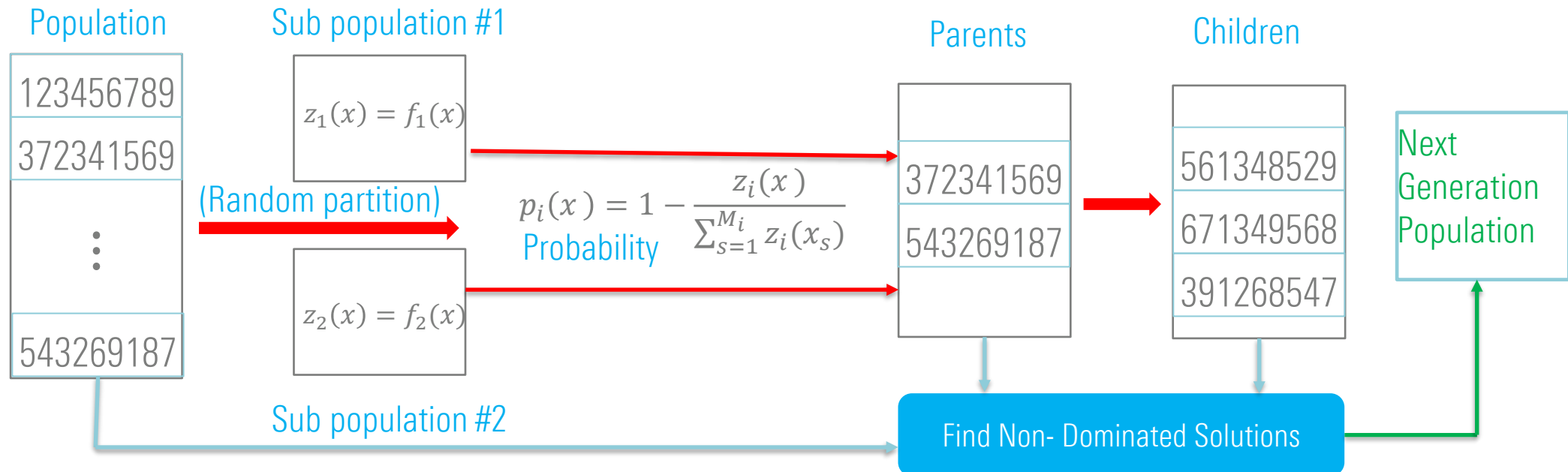
Method	Fitness Evaluation	Parent Selection	Elitism
VEGA (Schaffer, 1985)	Single objective	Probability distribution	Dominance relation
MOGA (Fonseca & Fleming, 1993)	Dominance relation	Probability distribution	NA
NSGA (Srinivas and Deb, 1994)	Dominance relation	Probability distribution	NA
NSGA-II (Debb, etc., 2002)	Dominance relation	Probability distribution	Dominance relation
NPGA (Horn, etc. , 1994)	No Fitness	Tournament method (dominance relation)	NA
PAES (Knowles and Corne, 1999)	No Fitness	Local search (dominance relation)	Dominance relation

Classification of Multi Objective Genetic Algorithms

- Dominance relation in Elitism
 - VEGA (Schaffer, 1985)
- Dominance relation in fitness function
 - MOGA (Fonseca & Fleming, 1993),
 - NSGA (Srinivas and Deb, 1994) ,
 - NSGA-II (Debb, etc., 2002)
- No fitness values, but dominance relation in selection/elitism process
 - NPGA (Horn, etc. , 1994),
 - PAES (Knowles and Corne, 1999)

Multi Objective Evolutionary Algorithms: VEGA

- Vector Evaluated Genetic Algorithm (VEGA¹)
 - First genetic algorithm applied to MOO: $\min_{x \in S} (f_1, f_2)$
 - Fitness value, $z_i(x)$, is based on objective function $f_i(x)$



1. Schaffer, 1985: *Multiple Objective Optimization with Vector Evaluated Genetic Algorithms*, The First International Conference on Genetic Algorithms and their Applications (held in Pittsburgh), pp. 93–100

Multi Objective Evolutionary Algorithms: MOGA

- Multi-Objective Genetic Algorithm (MOGA¹)

- Rank all solutions: $r(x) = 1 + (\# \text{ of solutions that dominates } x)$
- Fitness value:

$$z(x) = N - \sum_{k=1}^{r(x)-1} n_k - 0.5(n_{r(x)} - 1)$$

$N = 5$, Total number of solutions

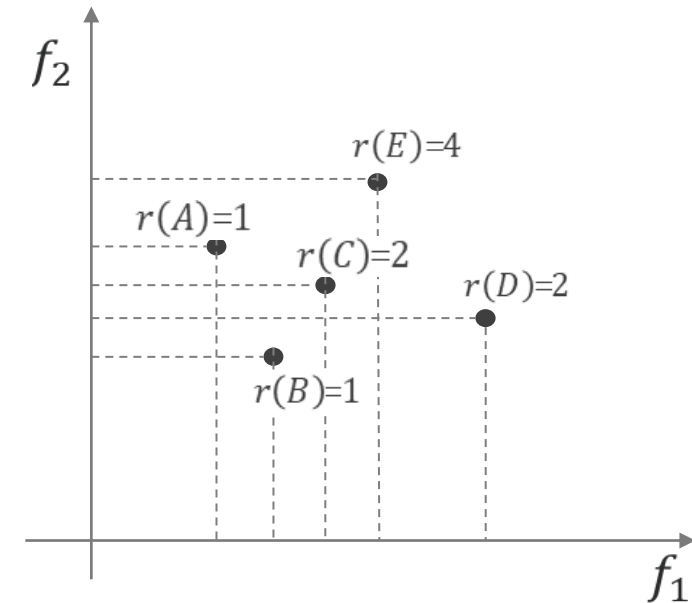
n_k = Number of solutions with $r(x) = k$:

$$n_1 = 2, \quad n_2 = 2, \quad n_3 = 0, \quad n_4 = 1$$

$$z(E) = 5 - (2 + 2) - 0.5(1 - 1) = 1$$

$$z(C) = z(D) = 5 - (1) - 0.5(2 - 1) = 3.5$$

$$z(A) = z(B) = 5 - 0 - 0.5(2 - 1) = 4.5$$



1. Fonseca and Fleming, 1993: *Multiobjective Genetic Algorithm*, IEEE colloquium on 'Genetic Algorithms for Control Systems Engineering' (Digest No. 1993/130), 28 May 1993. London, UK: IEE; 1993

Multi Objective Evolutionary Algorithms: NSGA

- Nondominated Sorting Genetic Algorithm (NSGA¹)

- Sorting by selecting non-dominated solutions without replacement each time:

$$P_0 = \{A, B\}, P_1 = \{C, D\}, P_2 = \{E\}$$

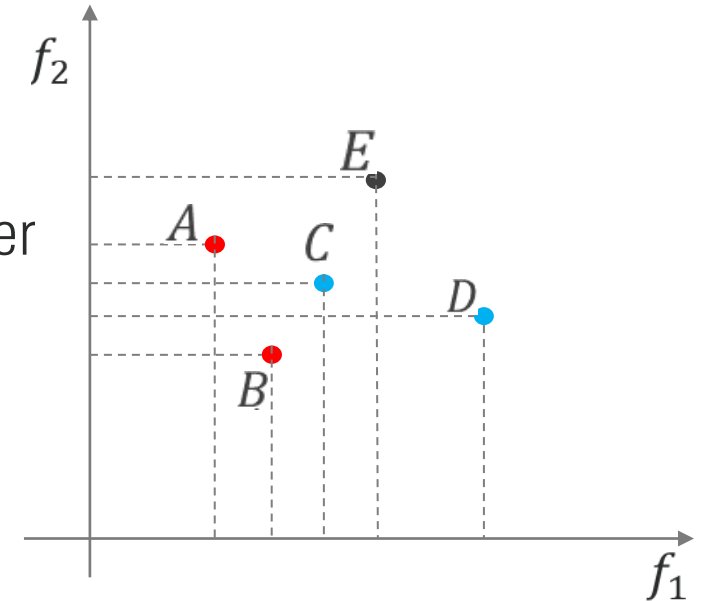
$$P_0 \text{ dominates } P_1 \text{ dominates } P_2$$

- Assign same fitness value $z(x)$ for each x in P_i based on order

$$P_0: z(A) = z(B) = 10$$

$$P_1: z(C) = z(D) = 8$$

$$P_2: z(E) = 5$$



1. Srinivas and Deb, 1994: *Multiobjective optimization using nondominated sorting in genetic algorithms*. Journal of Evolutionary Computing 1994;2(3):221–48.

Multi Objective Evolutionary Algorithms: NSGA-II

- Nondominated Sorting Genetic Algorithm II (NSGA-II¹)

- Sorting by number of dominated solutions

$$P_1 = \{A, B\}, \quad 0 \text{ dominated solution}$$

$$P_2 = \{C, D\}, \quad 1 \text{ dominated solution}$$

$$P_3 = \{\}, \quad 2 \text{ dominated solutions}$$

$$P_4 = \{E\}, \quad 3 \text{ dominated solutions}$$

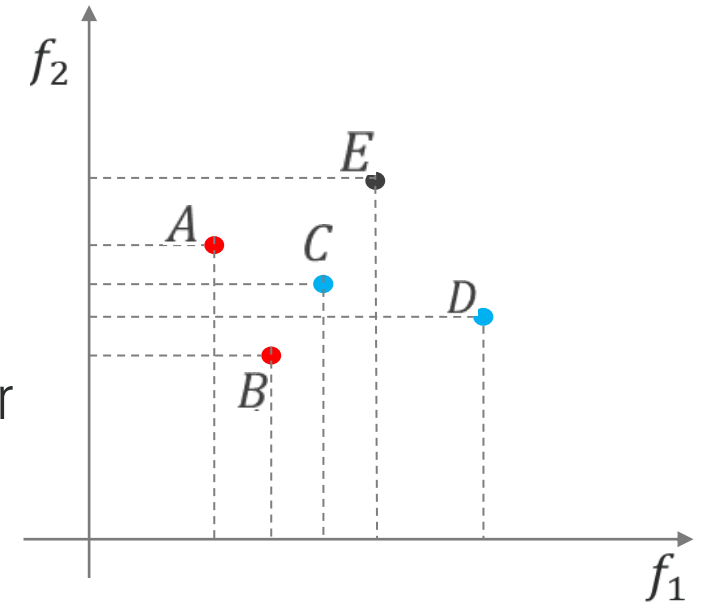
- Assign same rank value n_x for each x in P_i based on order

$$P_1: n_A = n_B = 1$$

$$P_2: n_C = n_D = 2$$

$$P_4: n_E = 3$$

- All solutions are ranked by pair (n_x, d_x) , d_x is a crowding distance



1. Deb, Pratap, Agarwal, Meyarivan, 2002: *A fast and elitist multiobjective genetic algorithm: NSGA-II*. IEEE Trans Evolutionary Computing 2002;6(2):182–97.

Multi Objective Evolutionary Algorithms: NPGA

- Niched Pareto Genetic Algorithm (NPGA¹)

- Use tournament method for Parent selection

Selection: for randomly pair $x, y \in P$,

randomly choose $G = \{C\}$

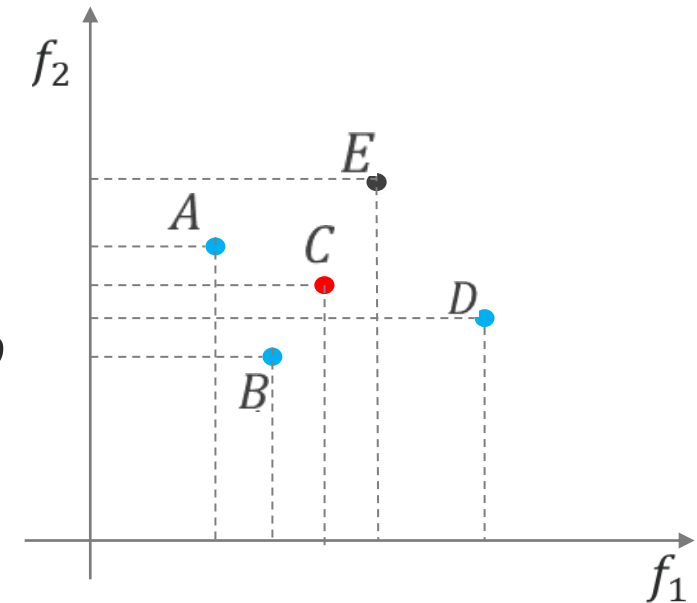
choose a 'better one' comparing with G :

(A, E) : E is dominated by G \rightarrow choose A

(B, E) : E is dominated by G \rightarrow choose B

(B, D) : neither B or D is dominated by G \rightarrow choose D
(D is in less crowded area)

Parent = $\{A, B, D\}$



1. Horn, Nafpliotis and Goldberg A, 1994: *A niched Pareto genetic algorithm for multiobjective optimization*. Proceedings of the first IEEE conference on evolutionary computation. IEEE world congress on computational intelligence, 27–29 June, Orlando, FL, USA, 1994.

Multi Objective Evolutionary Algorithms: PAES

■ Pareto Archived Evolution Strategy (PAES¹)

– Selection Operator

Archived Solutions: $G = \{\text{Non-Dominated Solutions discovered}\}$,
initialize $G = \emptyset$

Local Search:

Random select A_0 as a Parent, $G = \{A_0\}$

Mutate $A_0 \rightarrow A'_0$, dominated by A_0 , **discard** A'_0

Mutate $A_0 \rightarrow A_1$, dominates A_0 , be a new Parent

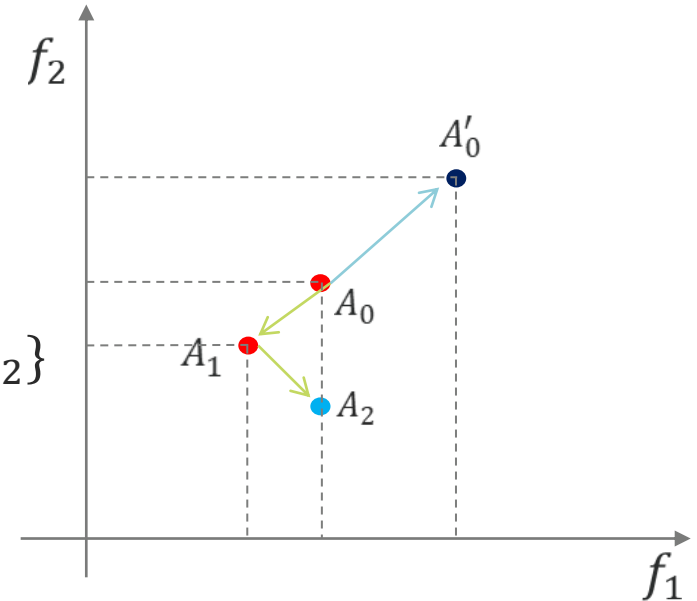
Mutate $A_1 \rightarrow A_2$, A_1 and A_2 are **equally 'good'**

Update Archive G :

Replace A_0 in G by a **better** A_2 (if A_2 dominates A_0) and $G = \{A_2\}$

or

Choose either A_1 or A_2 (based on crowdedness) to add to G
if A_2 does not dominate G



1. Knowles and Corne, 1999: *The Pareto archived evolution strategy: a new baseline algorithm for Pareto multiobjective optimization*. Proceedings of the 1999 congress on evolutionary computation, 6–9 July 1999. Washington, DC USA

Multi Objective Evolutionary Algorithms: Special Considerations

- Inherited weakness of EA
 - Converge towards **local optima** rather than the global optimum
- How to maintain solution diversity?
 - **Niche Count**¹: $nc(x)$
 - More crowded around x ➔ bigger $nc(x)$
 - **Fitness Sharing**¹: discount fitness value with niche count:

$$z'(x) = \frac{z(x)}{nc(x)}$$

1. David E. Goldberg, *Genetic Algorithms in Search, Optimization & Machine Learning*, Addison Wesley Publishing Company, 1989

Multi Objective Evolutionary Algorithms: Other EAs

- MOEA methods based on other EAs

- Particle Swarm Optimization (PSO)

James Kennedy and Russell C. Eberhart *Particle swarm optimization*. Proceedings of the 1995 IEEE International Conference on Neural Networks, Piscataway, New Jersey, 1995

M. Reyes-Sierra and C. Coello, *Multi-Objective Particle Swarm Optimizers: A Survey of the State-of-the-Art*, International Journal of Computational Intelligence Research, Vol.2, No.3 (2006), pp. 287–308

- Simulated Annealing (SA)

Paolo Serafini, *Simulated Annealing for Multi Objective Optimization Problems*, Multiple Criteria Decision Making, Springer-Verlag New York, Inc. 1994

- Ant Colony Optimal (ACO)

Marco Dorigo, Gianni Di Caro, *Ant Colony Optimization: A New Meta-Heuristic*, Proceedings of the 1999 Congress of Evolutionary Computation - CEC99

Algorithm Evaluation Based on Pareto Set

- What is a good approximation of Pareto Set
- Hypervolume Indicator¹ $H(A)$
 - $A = \{a_1, a_2, a_3, a_4\}$ is the solution set in objective space
 - r is the reference, [anti-utopia point](#) (worst of each objective)
 - $H(A)$ is [area covered by cubes](#) defined by a_i and r :

$$H(A) = \text{area}(\cup c(a_i, r))$$

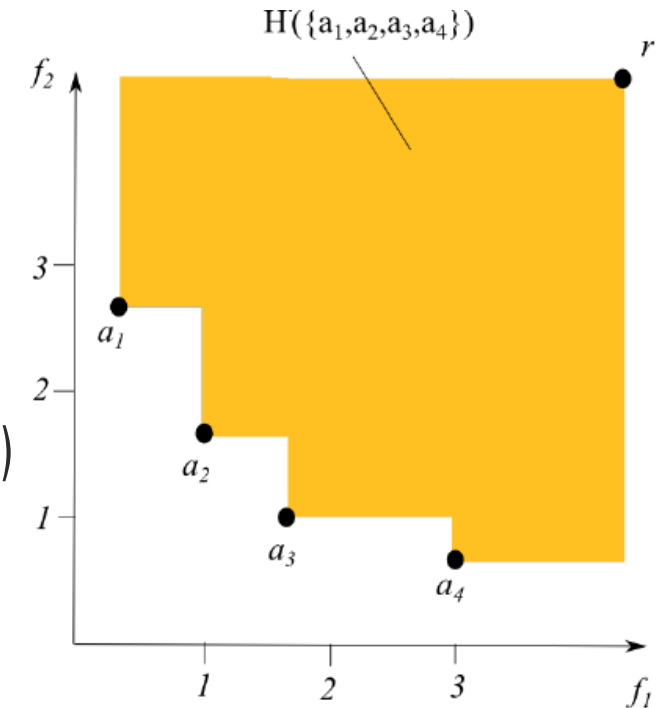


Image Source: [ResearchGate](#)

A bigger $H(A)$ represents a better solution set

1. Eckart Zitzler, Dimo Brockhoff, and Lothar Thiele, The Hypervolume Indicator Revisited: On the Design of Pareto-compliant Indicators Via Weighted Integration, EMO 2007, LNCS 4403, pp. 862–876, 2007.

Contents

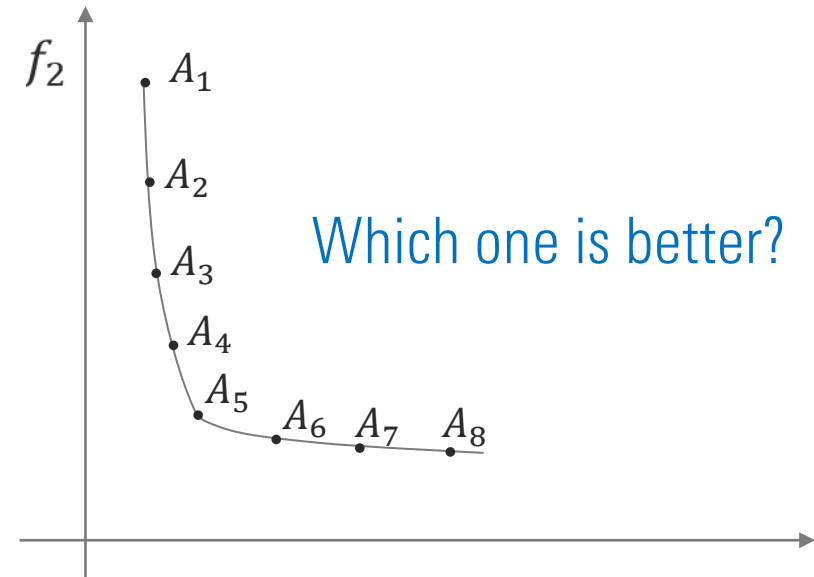
- Background and Some History
- Multi Objective Optimization (MOO)
- MOO Algorithms
 - Scalarization Algorithms
 - Multi Objective Evolutionary Algorithms
 - Algorithm Evaluation Based on Pareto Set
- Selection of a Single Solution in Pareto Set
- MOO Libraries
- Summary & QA

Selection of a Single Solution in Pareto Set: No DM Available

- When do we need to produce Pareto set?
 - Most MOEA method (A posterior, No DM available)
 - Scalarization without DM preference (A posterior, No DM available)
- Example: Recommender Systems balancing multi metrics
 - End user (DM) cannot choose from Pareto set
 - A single best recommendation list needs to be produced

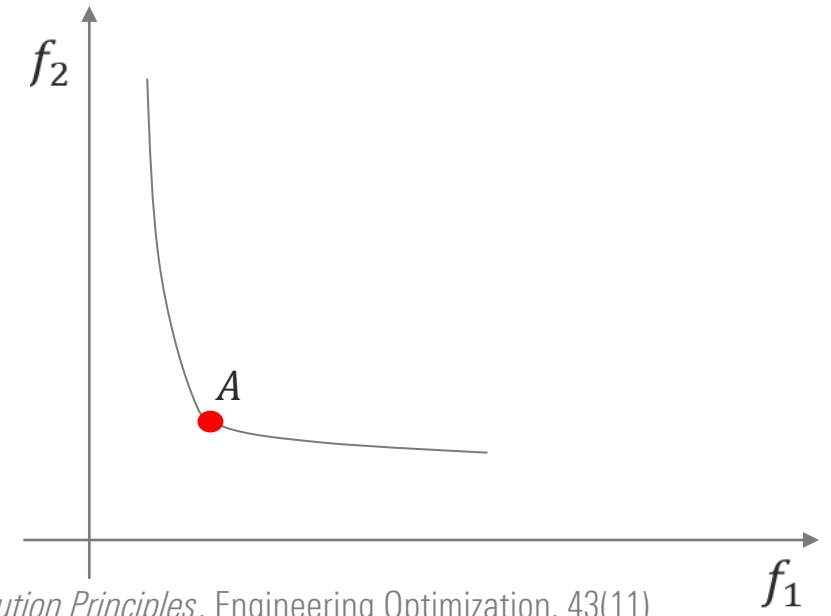
Selection of a Single Solution in Pareto Set: Best Guess

- No information from decision maker (DM)
 - All solutions in Pareto set are 'equally good'
 - Need to make the 'best' guess
- Best guess method
 - Knee point method
 - Hypervolume Method
 - Multiple-criteria decision-making (MCDM) methods



Selection of Single Solution in Pareto Set: Knee Point

- Knee Point
 - A special point (A) on Pareto Front
 - **small improvement** in either objective will **cause** a **large deterioration** in the other objective,
- Methods of Finding Knee Point
 - **Angle Based Method**¹
 - Marginal Utility Method¹
 - Hyperplane Normal Vector Method²



1. Deb and Gupta, *Understanding Knee Points in Bicriteria Problems and Their Implications as Preferred Solution Principles*, Engineering Optimization, 43(11)

2. Yu, Jin, Olhofer, A Method for a Posteriori Identification of Knee Points Based on Solution Density, 2018 IEEE Congress on Evolutionary Computation (CEC)

Selection of a Single Solution in Pareto Set: Angle Based Knee Point

■ Angle Based Knee Point¹

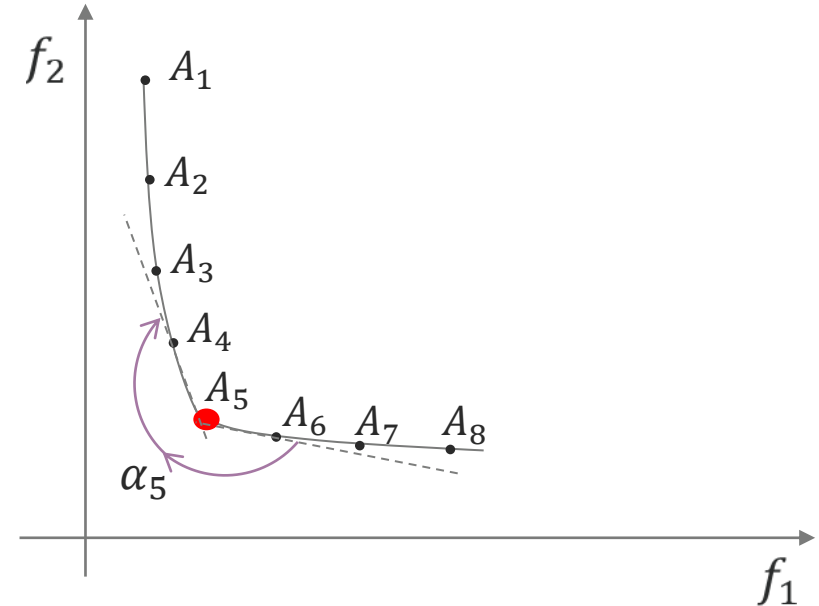
- Only work in **two objectives** M00
- Pareto front: $\{A_1, A_2, \dots, A_8\}$
- Calculate **reflex angle** α for each point:

$$\alpha_i = \angle A_{i-1}A_iA_{i+1}$$

- Find the point with $\max \alpha_i$

$$\alpha_5 = \max\{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, \alpha_7\}$$

A_5 is the **Knee point**



1. Deb and Gupta, *Understanding Knee Points in Bicriteria Problems and Their Implications as Preferred Solution Principles*, Engineering Optimization, 43(11)

Selection of a Single Solution in Pareto Set: Hypervolume Method

■ Hypervolume Method¹

- Define reference point r : worst of each objective (Upper Bound Point)

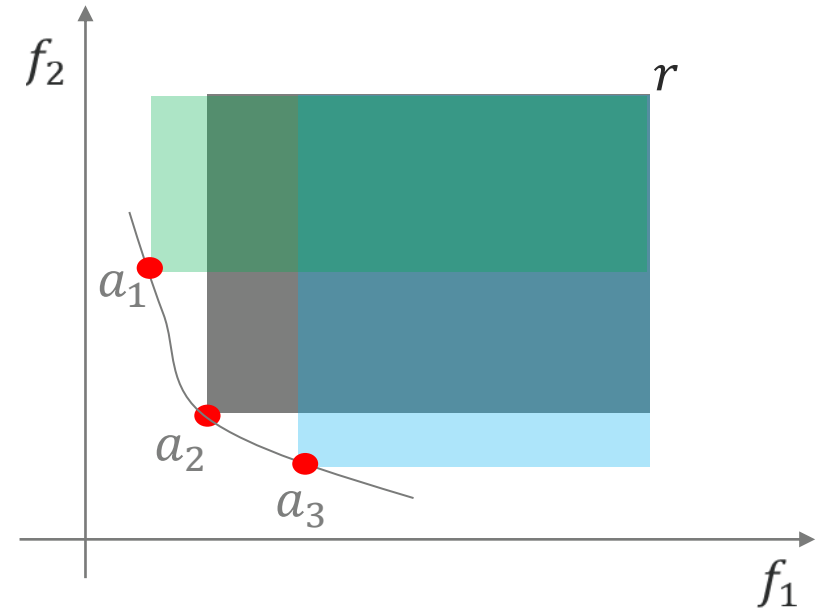
$$r = F^- = (f_1^-, f_2^-, \dots, f_M^-)$$

- Evaluate Hypervolume for each solution $\{a_i\}$:

$$H(a_i), i = 1, 2, \dots, N$$

- Best solution with max hypervolume

$$\arg \max_i H(a_i)$$



1. Eckart Zitzler, Dima Brockhoff, and Lothar Thiele, The Hypervolume Indicator Revisited: On the Design of Pareto-compliant Indicators Via Weighted Integration, EMO 2007, LNCS 4403, pp. 862–876, 2007.

Selection of a Single Solution in Pareto Set: MCDM Methods

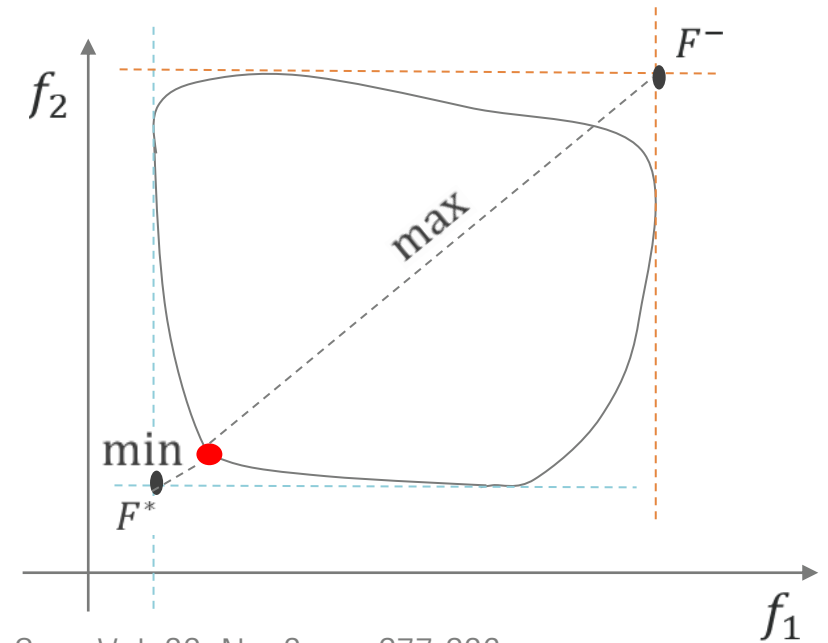
- Multiple-criteria decision-making (MCDM) methods¹:
 - Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS)
 - Preference Ranking Organization METHod for Enrichment of Evaluations (PROMETHEE)
 - Least misery method
 - ÉLimination et Choix Traduisant la REalité (ÉLECTRE)
 - ...
- Most MCDM methods still need DM preference

1. https://en.wikipedia.org/wiki/Multiple-criteria_decision_analysis

Selection of a Single Solution in Pareto Set: TOPSIS

- Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS¹)
 - A Pareto solution point: that is most close to ideal point or most apart to anti-ideal point
 - Utopia point: $F^* = (f_1^*, f_2^*, \dots, f_M^*)$
 - Upper bound point: $F^- = (f_1^-, f_2^-, \dots, f_M^-)$
 - Find best Solution x in Pareto set:

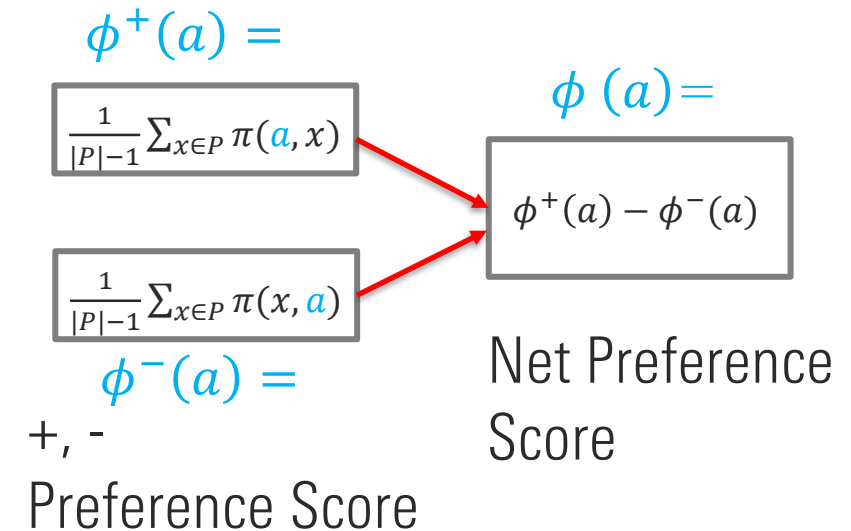
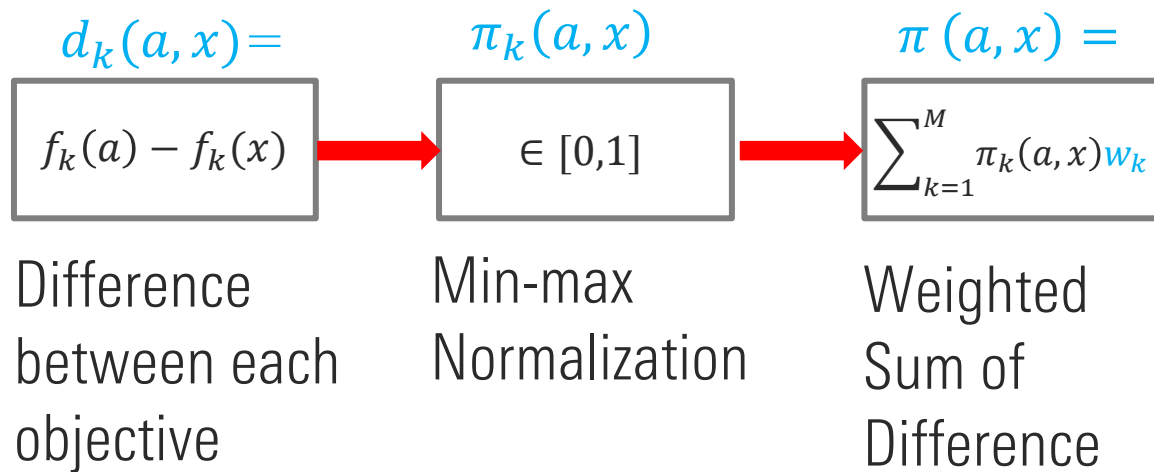
$$\min_x ||F(x) - F^*||$$
$$\max_x ||F(x) - F^-||$$



1. Kwangsun Yoon, *A Reconciliation among Discrete Compromise Solutions*, J. opl Res. Soc., Vol. 38, No. 3, pp. 277-286, 1987.

Selection of a Single Solution in Pareto Set: PROMETHEE

- Preference Ranking Organization METHod for Enrichment of Evaluations (PROMETHEE), e.g., pairwise ranking,



- Need weights for each objective

Contents

- Background and History
- Multi Objective Optimization (MOO)
- MOO Algorithms
 - Scalarization Algorithms
 - Multi Objective Evolutionary Algorithms
 - Algorithm Evaluation Based on Pareto Set
- Selection of a Single Solution in Pareto Set
- MOO Libraries
- Summary & QA

MOO Libraries

Name	MOO Methods	Single Objective	Language	Open Source	Last update	Link
PyGMO	NSGA-II, MOEA, MH-AOC, NS-PSO	Yes	Python	Yes	2021	https://esa.github.io/pygmo2/index.html
pymoo	NSGA-II, NSGA-III, MOEA	Yes	Python	Yes	2022	https://pymoo.org/
Inspired	PAES, NSGA-II	Yes	Python	Yes	2019	https://pythonhosted.org/inspired/
Platypus	NSGA-II, MOEA, SPEA2, MOEA/D, PSO, PAES, PESA2	No	Python	Yes	2022	https://platypus.readthedocs.io/
MOEA Framework	NSGA-II, NSGA-III, PAES, PESA2, SPEA2, MOEA, MO-PSO	Yes	Java	Yes	2022	http://moeaframework.org/
MATLAB & Simulink	MOEA, NSGA, SPEA2	Yes	Matlab	No	2021	https://www.mathworks.com/matlabcentral/fileexchange
openGA	NSGA-III	Yes	C++	Yes	2020	https://github.com/Arash-codedev/openGA

MOO Libraries: pymoo demo (https://pymoo.org/getting_started/index.html)

- Define Problem:

$$\begin{aligned} \min \quad & f_1(x) = 100(x_1^2 + x_2^2) \\ \min \quad & f_2(x) = (x_1 - 1)^2 + x_2^2 \\ \text{s.t.} \quad & g_1(x) = 2(x_1 - 0.1)(x_1 - 0.9) / 0.18 \leq 0 \\ & g_2(x) = -20(x_1 - 0.4)(x_1 - 0.6) / 4.8 \leq 0 \\ & -2 \leq x_1 \leq 2 \\ & -2 \leq x_2 \leq 2 \\ & x \in \mathbb{R} \end{aligned}$$



- Initiate the MOO Algorithm

```
from pymoo.algorithms.moo.nsga2 import NSGA2
from pymoo.operators.crossover.sbx import SBX
from pymoo.operators.mutation.pm import PM
from pymoo.operators.sampling.rnd import FloatRandomSampling

algorithm = NSGA2(
    pop_size=40,
    n_offsprings=10,
    sampling=FloatRandomSampling(),
    crossover=SBX(prob=0.9, eta=15),
    mutation=PM(eta=20),
    eliminate_duplicates=True
)
```

```
import numpy as np
from pymoo.core.problem import ElementwiseProblem

class MyProblem(ElementwiseProblem):

    def __init__(self):
        super().__init__(n_var=2,
                          n_obj=2,
                          n_ieq_constr=2,
                          xl=np.array([-2, -2]),
                          xu=np.array([2, 2]))

    def _evaluate(self, x, out, *args, **kwargs):
        f1 = 100 * (x[0]**2 + x[1]**2)
        f2 = (x[0]-1)**2 + x[1]**2

        g1 = 2*(x[0]-0.1) * (x[0]-0.9) / 0.18
        g2 = - 20*(x[0]-0.4) * (x[0]-0.6) / 4.8

        out["F"] = [f1, f2]
        out["G"] = [g1, g2]

problem = MyProblem()
```

MOO Libraries: pymoo demo (https://pymoo.org/getting_started/index.html)

- Define Termination Condition:

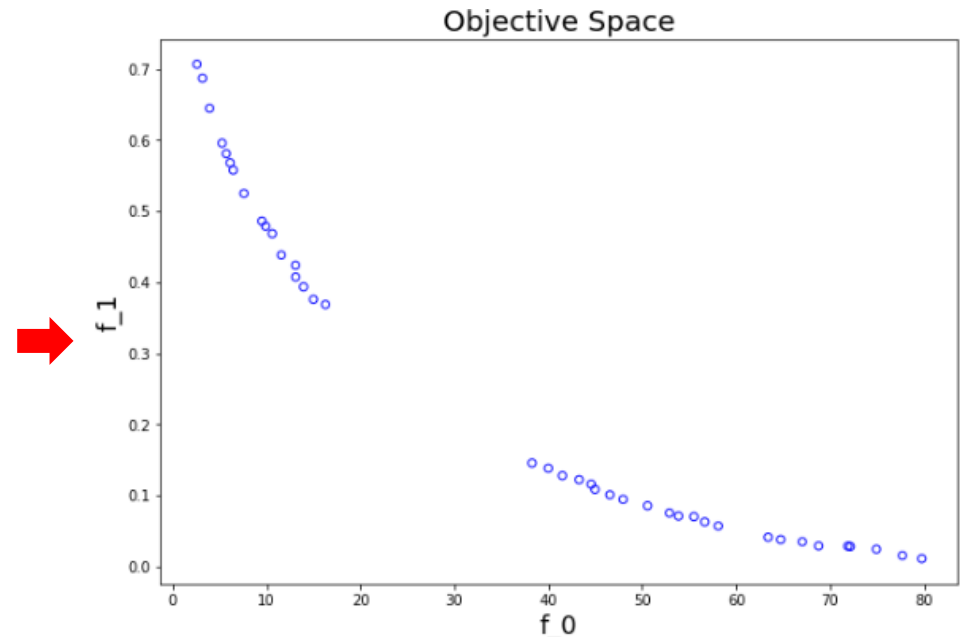
```
from pymoo.termination import get_termination
termination = get_termination("n_gen", 40)
```

- Run Optimizer:

```
from pymoo.optimize import minimize

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

# save results for later analysis
X = res.X # Pareto Set
F = res.F # Pareto Front
hist = res.history # running history
```



MOO Libraries: pymoo demo (https://pymoo.org/getting_started/index.html)

- Convergence: Collect history data

```
| n_evals = []           # corresponding number of function evaluations|
| hist_F = []           # the objective space values in each generation|
|
| for algo in hist:
|
|     # store the number of function evaluations
|     n_evals.append(algo.evaluator.n_eval)
|
|     # retrieve the optimum from the algorithm
|     opt = algo.opt
|
|     # filter out only the feasible and append and objective space values
|     feas = np.where(opt.get("feasible"))[0]
|     hist_F.append(opt.get("F")[feas])
```

MOO Libraries: pymoo demo (https://pymoo.org/getting_started/index.html)

■ Convergence: Check Hypervolume

```
# used for normalization of objective
approx_ideal = F.min(axis=0)
approx_nadir = F.max(axis=0)

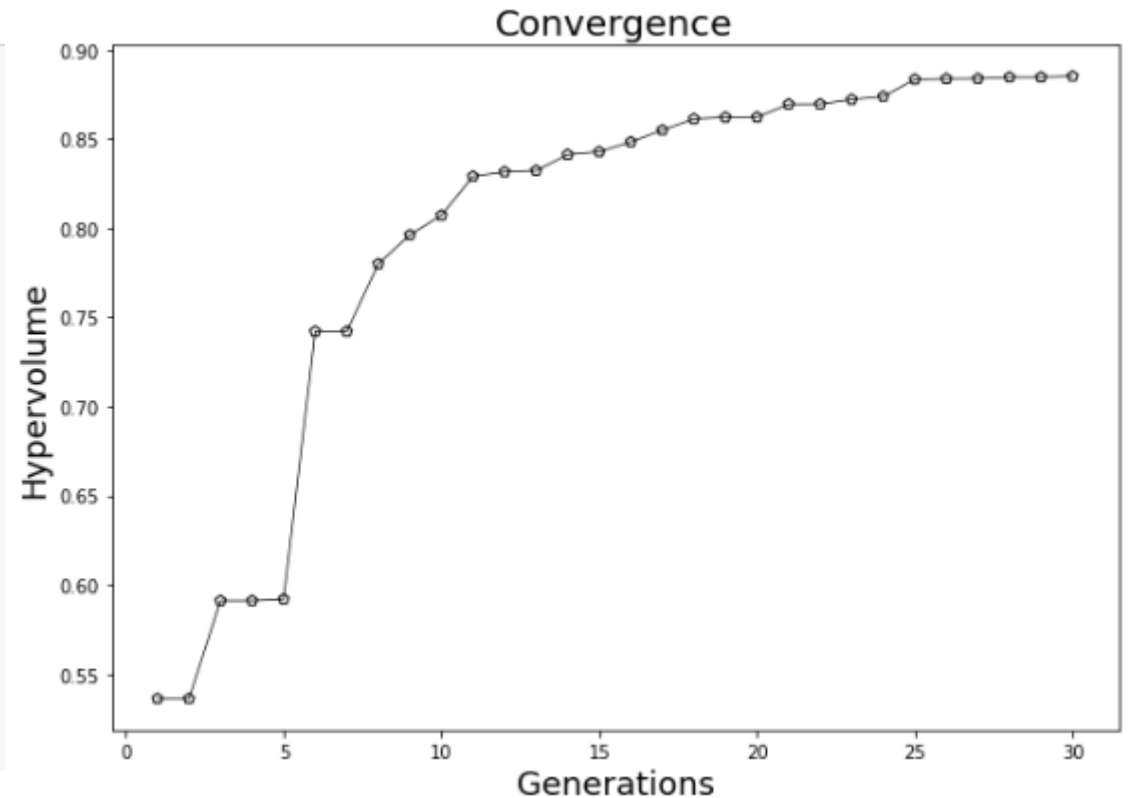
ref_point = np.array([1.1, 1.1])

from pymoo.indicators.hv import Hypervolume

metric = Hypervolume(ref_point=ref_point,
                     norm_ref_point=False,
                     zero_to_one=True,
                     ideal=approx_ideal,
                     nadir=approx_nadir)

hv = [metric.do(_F) for _F in hist_F]

plt.figure(figsize=(10, 7))
plt.plot(range(1, len(n_evals) + 1), hv, color='black', lw=0.7, label="Avg. CV of Pop")
plt.scatter(range(1, len(n_evals) + 1), hv, facecolor="none", edgecolor='black', marker="p")
plt.title("Convergence", fontsize=20)
plt.xlabel("Generations", fontsize=18)
plt.ylabel("Hypervolume", fontsize=18)
plt.show()
```



Summary, Q&A

- The solution of MOO problem must be **Pareto Optimal**
- **A Pareto Set** must be found if DM preference is not available
 - **Multiple runs** of Scalarization algorithms is needed to get Pareto set
 - **A single run** of Evolutionary Algorithms can get Pareto set
 - **Evenly distributed** Pareto set is needed
- **One 'best' solution** should be identified in Pareto set for DM in most cases