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Journal of Applicable Chemistry

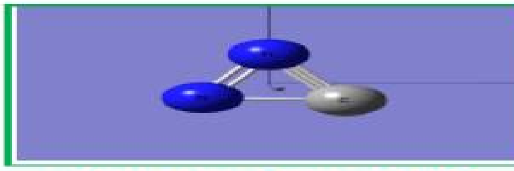
2018, 7 (4): 1084-1120

(International Peer Reviewed Journal)

New Chemistry News

$^{-}$N=C=N^{-}

New News of Chem (NNC)



ChemNewsNew (CNN)

Pareto optimality in Omni_metrics (Om)

Binary Hybrid Algorithms of Pareto Strategy

Mathematical Space

PSO + Pareto

Multi-objective Particle Swarm Optimization Hybrid Algorithm: An Application on Industrial Cracking Furnace

Ind. Eng. Chem. Res., 2007, 46 (11), 3602–3609
DOI: 10.1021/ie051084t

- Task: [naphtha industrial cracking furnace]
- MultiObjectFns: [yield rates [ethylene ; propylene]].
- decision variables :[ratio of gas to hydrocarbon, coil outlet temperature (COT) of pyrolysis gas, outlet pressure]
- Method : [multi-objective particle swarm optimization (MOPSO) + Pareteo]
- Alg.: Calculate Pareto set as a repository of particles
- use later by other particles to guide their own flight
- MOPSO + ANN hybrid model →
- for operation optimization of a naphtha industrial cracking furnace

Chengfei Li, Qunxiong Zhu, and Zhiqiang Geng

Multi-objective particle swarm optimization (MOPSO) procedure,

- + better convergence
- + diversity Pareto solutions than the NSGAII algorithm

Optimization of Adiabatic Styrene Reactor: A Hybrid Multiobjective Differential Evolution (H-MODE) Approach

Ind. Eng. Chem. Res., 2009, 48 (24), 11115–11132
DOI: 10.1021/ie901074k

- Soln.Method: [global search: evolutionary algorithm + local search: deterministic alg.]
- The proposed algorithm converges to a better set of nondominated solutions (possibly a Pareto front) as compared to the nondominated solutions obtained using NSGA and an improved strategy of MODE algorithm
-
- benchmark test fn: (KUR) : compared algs in
- Task2: [multiobjective optimization of an industrial adiabatic styrene reactor]
- Soln: with prevalidated model using the hybrid-MODE algorithm and an improved strategy of MODE.
- Four cases (three sets of two-objective optimization, cases 1−3, and one set of three-objective optimization, case 4) are considered consisting of

Hybrid Artificial Neural Network−Genetic Algorithm Technique for Modeling and Optimization of Plasma Reactor

Ind. Eng. Chem. Res., 2006, 45 (20), 6655–6664
DOI: 10.1021/ie060562c

- Task: [dielectric barrier discharge (DBD) plasma reactor without catalyst and heating]
- Model: hybrid artificial neural network−genetic algorithm for simulation, and optimization
- Effects of CH_4/CO_2 feed ratio, total feed flow rate, and discharge voltage on the performance of noncatalytic DBD plasma reactor were studied by an ANN-based simulation with a good fitting.
- Tasks: CH_4 conversion and C_{2+} selectivity, CH_4 conversion and C_{2+} yield, CH_4 conversion and H_2 selectivity
- X: [feed flow rates of the three initiators and of the transfer agent, inlet temperature, inlet pressure, average temperatures of the fluids in the five jackets]
- Constraints: [temperature of the reaction mass is constrained to lie below a safe value; equality constraint for the number-average molecular weight ($M_{n,f}$) of the product, to ensure product quality]
- Pareto-optimal solutions are obtained.
- Method: binary-coded NSGA-II-aJG and NSGA-II-JG
  - + perform better than NSGA-II near the hard end-point constraints

Istadi, and N. A. S. Amin

Jumping genes + Pareto

Multi-objective Optimization of the Operation of an Industrial Low-Density Polyethylene Tubular Reactor Using Genetic Algorithm and Its Jumping Gene Adaptations

Ind. Eng. Chem. Res., 2006, 45 (9), 3182–3199
DOI: 10.1021/ie050977i

- Task: [LDPE reactor]
- ConflObject: [max(monomer conversion) ; min (sum of normalized concentrations of three important side products (methyl, vinyl, and vinylidene groups)]
- Methods: binary-coded non-dominated sorting genetic algorithm
  - ® NSGA-II,
  - ® NSGA-II-JG,
  - ® NSGA-II-aJG

Naveen Agrawal, G. P. Rangaiah, Ajay K. Ray, and Santosh K. Gupta

SAA + Pareto

Development of a Robust Multiobjective Simulated Annealing Algorithm for Solving Multiobjective Optimization Problems

Ind. Eng. Chem. Res., 2011, 50 (11), 6728–6742
DOI: 10.1021/ie1016859

- Task: [computationally intensive and simulation-intensive MOO problems in chemical technology/ engineering fields of
- Robust multiobjective simulated annealing (rMOSA): rMOSA is a simulated annealing based multiobjective optimization algorithm
  - + speeds up the process of convergence to attain Pareto front (or a set of nondominating solutions)
  - + uniform non-dominating solutions along final Pareto front obtained
- NSGA-II-JG and NSGA-II
- best algorithm for solving

+ rMOSA is proved to converge to Pareto sets in less number of simulations with well-crowded uniform nondominating solutions in them

B. Sankararao and Chang Kyoo Yoo

DiffEvol + Pareto

Optimization of Adiabatic Styrene Reactor: A Hybrid Multiobjective Differential Evolution (H-MODE) Approach

Ind. Eng. Chem. Res., 2009, 48 (24), pp 11115–11132
DOI: 10.1021/ie901074k

- benchmark test fn: (KUR): compared algs in
- Task2: [multiobjective optimization of an industrial adiabatic styrene reactor]
- Soln: with prevalidated model using the hybrid-MODE algorithm and an improved strategy of MODE.

Four cases (three sets of two-objective optimization, cases 1−3, and one set of three-objective optimization, case 4) are considered consisting of

Multi(m) ObjFns	Test case
two-	1−3
Three-	4

- Simultaneous maximization of styrene productivity, selectivity, yield
  - four decision variables
  - two constraints
- hybrid strategy of MODE converges to the true Pareto front more rapidly (in fewer function evaluations) → well-diversified Pareto front as compared to the stand-alone evolutionary approach

Ashish M. Gujarathi and B. V. Babu

Hybrid Modeling of Methane Reformers. 3. Optimal Geometries of Perforated Catalyst Pellets

Ind. Eng. Chem. Res., 2009, 48 (23), 10277–10283
DOI: 10.1021/ie9001662

- ConflObject: [maximization (specific area); minimum (wall thickness of the pellet) simultaneous maximization (overall catalyst activity in the catalyst bed); minimum wall thickness of the pellet)]
- Pareto filter: ObJFns evaluated for several catalyst geometries
- The Pareto fronts obtained for the two analyzed cases are essentially the same
- Inference: maximization of the specific area constitutes a useful criterion for design of perforated catalysts in diffusion-controlled systems

André L. Alberton, Marcio Schwaab, Roberto Carlos Bittencourt, Martin Schmal and José Carlos Pinto

Hierarchical Pareto

Hierarchical Pareto Optimization for the Sustainable Development of Industrial Ecosystems

Ind. Eng. Chem. Res., 2006, 45 (9), 3265–3279
DOI: 10.1021/ie050487q

- Hierarchical Pareto Optimization Methodology
  - + achieves most sustainable solution.
  - + systematic and flexible framework
  - + solves multiscale, multidimensional problems
  - + provides guidance for improving sustainability.

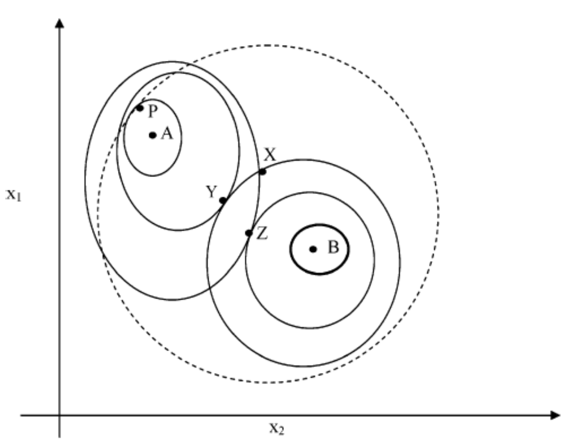
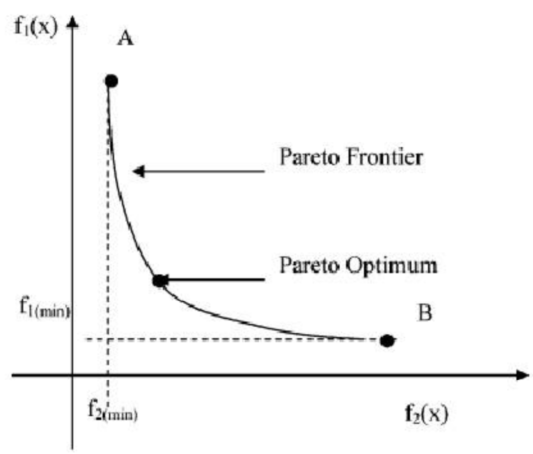


Illustration of Pareto optimum points (design space).



Pareto optimum (objective space

Aditi Singh, and Helen H. Lou

Parameters-- Precision & Correlation

Multiobjective Framework for Model-based Design of Experiments to Improve Parameter Precision and Minimize Parameter Correlation

Ind. Eng. Chem. Res., 2013, 52 (24), 8289–8304
DOI: 10.1021/ie400133m

- Multiobjective optimization
- Model based experimental design
- Pareto-optimal front
  - trade-off between system information and correlation among parameters

Vaibhav Maheshwari, Gade Pandu Rangaiah, and Lakshminarayanan Samavedham

Data Driven modeling

Data Driven Modeling Using an Optimal Principle Component Analysis Based Neural Network and Its Application to a Nonlinear Coke Furnace

Ind. Eng. Chem. Res., 2018, 57 (18), 6344–6352
DOI: 10.1021/acs.iecr.8b00071

- PCA; RBF-NN;
- NSGA II

Ridong Zhang , Qiang Lv, Jili Tao, and Furong Gao

Optimum Pareto Front

Application and Analysis of Methods for Selecting an Optimal Solution from the Pareto-Optimal Front obtained by Multiobjective Optimization

Ind. Eng. Chem. Res., 2017, 56 (2), 560–574
DOI: 10.1021/acs.iecr.6b03453

- 10 methods TO select optimal solution from the Pareto-optimal front
- MS Excel-based program.

Zhiyuan Wang and Gade Pandu Rangaiah

Optima and extrema
(Mathematical to physico-chemical-biological space)

- Optimization of reacting systems to a
  - Unique single, set of equivalent multiple, Pareto optimal group or a single Pareto optimal (the best, nearer to true value if known) solution(s) also
- evolved with human needs and progressive scientific pursuit.

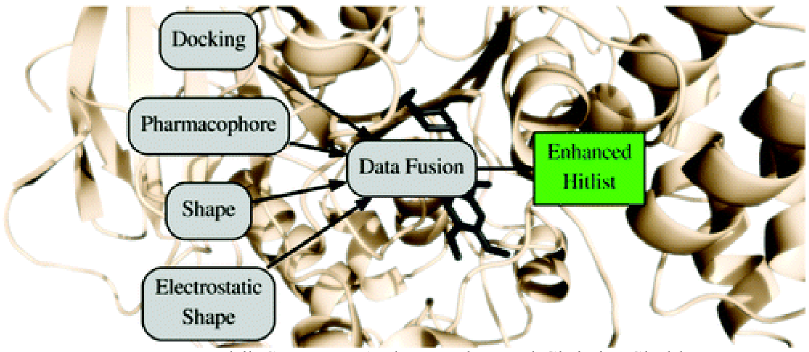
- The interactions are
  - physical, chemical and/or biological
    - in normal energy scale or very low/very high or even at extreme limits on planet earth or universe.
-
- From another perspective, interactions are among
  - matter with matter and/or energy, or energy with energy.
- Probing more and more is to
  - understand, control, alter the (natural/man made) phenomena for
    - befit of man- kind, other life forms and environment

Chemisty for Life — Drug research

Virtual Screening Data Fusion Using Both Structure- and Ligand-Based Methods

J. Chem. Inf. Model., 2012, 52 (1), 225–232
DOI: 10.1021/ci2004835

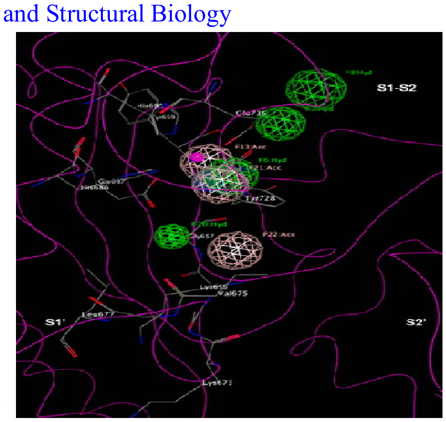
- DataGeneration: [docking, pharmacophore search, shape similarity, electrostatic similarity, spanning both structure- and ligand-based procedures]
- DataSets: 16
- DataFusionAlg: [sum rank, rank vote, sum score, Pareto ranking, parallel selection]



Fredrik Svensson, Anders Karlén, and Christian Sköld

Development of a Comprehensive, Validated Pharmacophore Hypothesis for Anthrax Toxin Lethal Factor (LF) Inhibitors Using Genetic Algorithms, Pareto Scoring, and Structural Biology

J. Chem. Inf. Model., 2012, 52 (7), 1886–1897
DOI: 10.1021/ci300121p



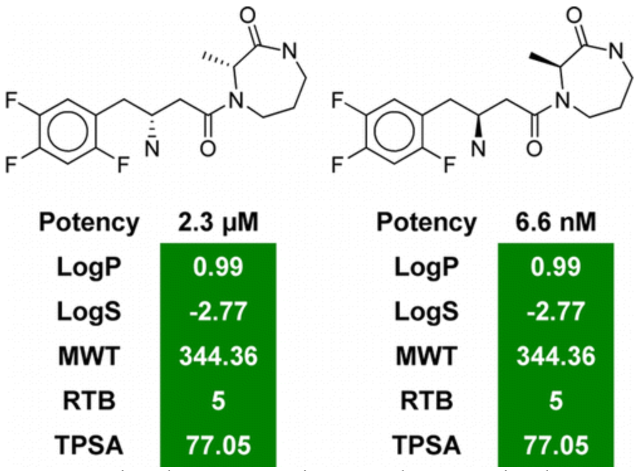
Ting-Lan Chiu and Elizabeth A. Amin

SAR

Multiobjective Particle Swarm Optimization: Automated Identification of Structure–Activity Relationship-Informative Compounds with Favorable Physicochemical Property Distributions

J. Chem. Inf. Model., 2012, 52 (11), 2848–2855

- Pareto-Optim(multipleObjFns)
  - + does not require subjective intervention.
  - + automated and can be easily modified.
- Case Study: screen 10 compound data sets of different composition and global SAR phenotypes



Vigneshwaran Namasivayam and Jürgen Bajorath

SPR	SVR	Descriptors

Quantitative Structure–Property Relationship Predictions of Critical Properties and Acentric Factors for Pure Compounds

J. Chem. Eng. Data, 2015, 60 (5), 1377–1387
DOI: 10.1021/je501093v

- 900 Compounds ; #Descp : 500;
- #Descip_final model for Tc::33;
- #Descip_final model for Pr::30;

Wendy Hawley Carande, Andrei Kazakov, Chris Muzny, and Michael Frenkel

Phospholipids **FFD** **MALDI-TOF_MS**

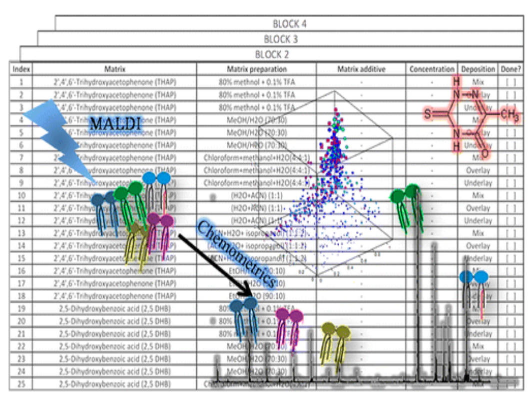
Fractional Factorial Design (FrFD) of MALDI-TOF-MS Sample Preparations for the Optimized Detection of Phospholipids and Acylglycerols

Anal. Chem., 2016, 88 (12), 6301–6308
DOI: 10.1021/acs.analchem.6b00512

- Computational-analytical optimization
- Analysis five lipids (4 phospholipids + 1 acylglycerol)
- Pareto optimality of experimental factors (FrFD)
  - Matrices,

matrix preparations, matrix additives, additive concentrations, and deposition methods →

- 8064 possible analyses →720 identified
:



Najla AlMasoud, Elon Correa, Drupad K. Trivedi, and Royston Goodacre

Sampling Multiple Scoring Functions Can Improve Protein Loop Structure Prediction Accuracy

J. Chem. Inf. Model., 2011, 51 (7), 1656–1666
DOI: 10.1021/ci200143u

- prediction of loop structures of proteins
- Pareto optimal sampling: to sample the function space of multiple scoring functions
- +tolerates insensitivity and inaccuracy in individual scoring functions → lead to significant accuracy improvement in loop structure prediction
- Output: ensemble of diversified structures yielding Pareto optimality to all sampled conformations.

- Application: POS method applied to a set of 4–12-residue loop targets using a function space composed of backbone-only Rosetta and distance-scale finite ideal-gas reference (DFIRE). 501 out of 502 targets, the model sets generated by POS contain structure models are within subangstrom resolution.
- developed Pareto optimal consensus (POC) method

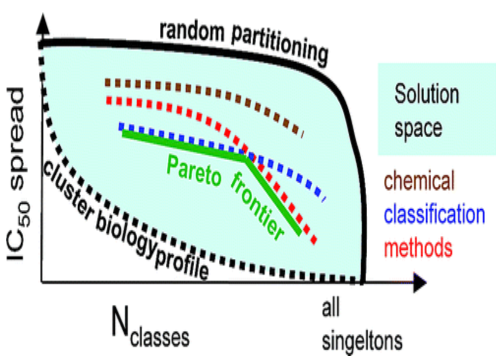
Yaohang Li, Ionel Rata, and Eric Jakobsson

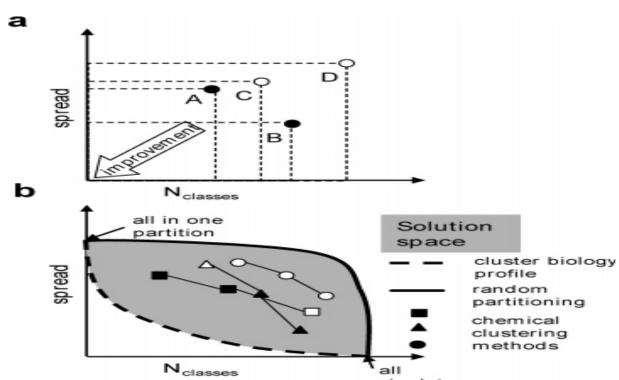
Clustering and Rule-Based Classifications of Chemical Structures Evaluated in the Biological Activity Space

J. Chem. Inf. Model., 2007, 47 (2), 325–336
DOI: 10.1021/ci6004004

® No classification method is overall superior to all others

- + Natural Way out: rule-based, scaffold-oriented methods are the better
- + If classes with homogeneous biological activity are required,
- + Then large number of clusters should be tolerated.
- + If fewer and larger classes are required, and some loss of homogeneity in biological activity is acceptable
- + Then clustering based on chemical fingerprints is superior





Ansgar Schuffenhauer, Nathan Brown, Peter Ertl, Jeremy L. Jenkins, Paul Selzer, and Jacques Hamon

Improving predicted protein loop structure ranking using a Pareto-optimality consensus method

BMC Structural Biology 2010, 10:22, 2-14

- Integrating multiple knowledge- and physics-based scoring functions
- Pareto Optimality Consensus (POC) Method
  - Basis: Pareto optimality + fuzzy dominance
  - Jacobson's loop decoy sets, membrane protein loop decoy sets
- selection accuracy: rank-by-vote, rank-by-number, rank-by-rank, and regression-
- Distinguishing the best loop models from others within a loop model set.

Yaohang Li, Ionel Rata, See-wing Chiu and Eric Jakobsson

Instrumental Probes

Liquid Chromatography

Comprehensive Study on the Optimization of Online Two-Dimensional Liquid Chromatographic Systems Considering Losses in Theoretical Peak Capacity in First- and Second-Dimensions: A Pareto-Optimality Approach

Anal. Chem., 2010, 82 (20), 8525–8536
DOI: 10.1021/ac101420f

- MultiObjectFns: [total analysis time, total peak capacity, total dilution]
- Instrument: [two-dimensional liquid chromatography]
- Model: Pareto-optimality →
- optimal parameters: [column particle sizes, column diameters, modulation times]

+ Accounted for losses in the peak capacities in the first dimension (due to undersampling) and in the second dimension (due to high injection volumes).
  - The first effect (detection band broadening) reduces the original peak capacity by about a half, the second effect can reduce the total peak capacity by an additional half.

G. Vivó-Truyols, Sj. van der Wal, and P. J. Schoenmakers

Approximate and Exact Equations for Peak Capacity in Isocratic High-Pressure Liquid Chromatography

Anal. Chem., 2011, 83 (20), 7614–7615
DOI: 10.1021/ac202102s

- Instru.chromatograph: [extra-column and column broadening on isocratic peak capacity]

- Pareto-Optimality Approach
  Vivo-Truyols, G.; van der Wal, Sj.; Schoenmakers, P. J. Anal. Chem.2010, 82, 8525–8536.

Peter W. Carr

Taguchi's Design	removal of Cd, Ni, Zn	Pareto analysis of variance	

Multicomponent Adsorption Study of Metal Ions onto Bagasse Fly Ash Using Taguchi's Design of Experimental Methodology

Ind. Eng. Chem. Res., 2007, 46 (17), 5697–5706
DOI: 10.1021/ie0609822

- Task: [opt parameters (simultaneous removal of Cd, Ni, and Zn metal ions from aqueous solutions using bagasse fly ash (BFA) as an adsorbent)]
- Method.ExptDes: Taguchi optimization methodology (L27 orthogonal array);
- X : [initial metal concentrations (C0,i), temperature, initial pH, adsorbent dosage (m), contact time on the adsorption of metal ions]; # levels : three
- y response: [(total amount of metal adsorbed on BFA, in terms of mg/g of BFA (qtot))]
- **Pareto analysis of variance →**
- Inference:
  - [most significant parameter: adsorbent dosage with 53.14% and 31.25% contribution to the qtot and signal-to-noise (S/N) ratio data
  - significantPar: interactions between the C0,i values]
- Confirmation experiments with Taguchi optimum operating conditions

Vimal C. Srivastava, Indra D. Mall, and Indra M. Mishra

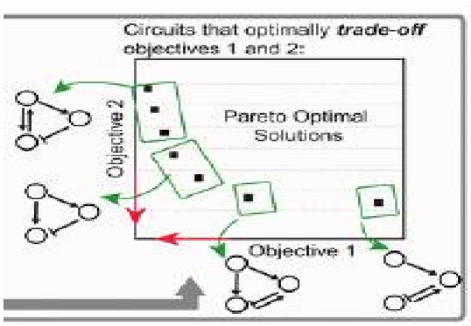
Biological Space

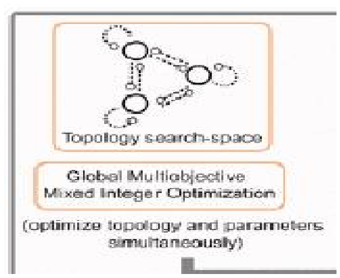
Synthetic Biology

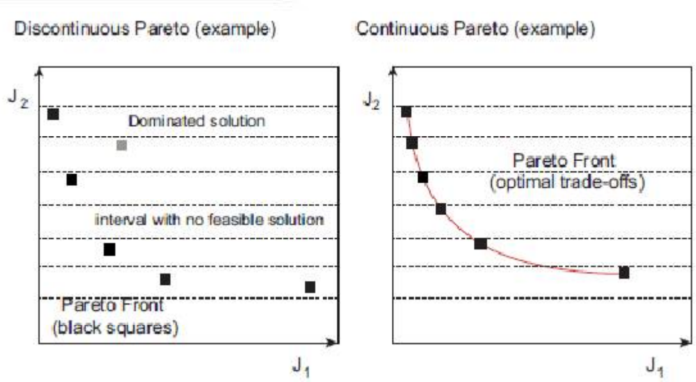
Automated Design Framework for Synthetic Biology Exploiting Pareto Optimality

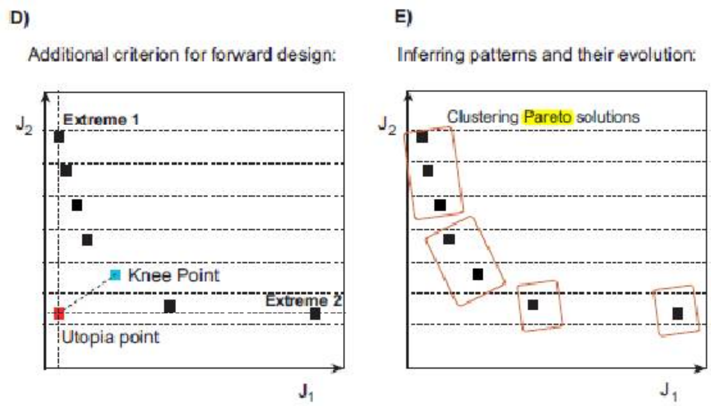
ACS Synth. Biol., 2017, 6 (7), 1180–1193
DOI: 10.1021/acssynbio.6b00306

- Gene regulatory networks motifs--for stripe formation, rapid adaption, fold-change detection







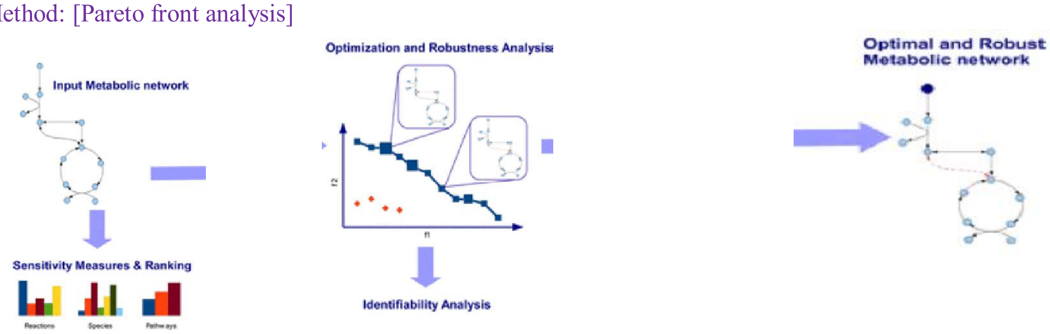


Irene Otero-Muras and Julio R. Banga

Efficient Behavior of Photosynthetic Organelles via Pareto Optimality, Identifiability, and Sensitivity Analysis

ACS Synth. Biol., 2013, 2 (5), 274–288
DOI: 10.1021/sb300102k

- Object: [maximize the CO2 uptake rate ; production of metabolites of industrial interest or for ecological purposes]
- Method: [Pareto front analysis]



Giovanni Carapezza, Renato Umeton, Jole Costanza, Claudio Angione¶, Giovanni Stracquadanio, Alessio Papini||, Pietro Lió¶, and Giuseppe Nicosia

Chemical Technology Space

Process Chemistry

Efficient Implementation of the Normal Boundary Intersection (NBI) Method on Multiobjective Optimization Problems

Ind. Eng. Chem. Res., 2001, 40 (2), pp 648–655
DOI: 10.1021/ie000400v

- Task: [chemical process simulator];
- Normal boundary intersection (NBI) + Summation of weighted objective functions (SWOF)

Young Il Lim, Pascal Floquet, and Xavier Joulia

Pareto Profile Benchmark for Kinetics of Filtration and Extent of Dewatering of Fine and Colloidal Suspensions

Ind. Eng. Chem. Res., 2005, 44 (24), pp 9364–9368
DOI: 10.1021/ie050605+

- .Pareto optimum, -- any improvement in the filtration kinetics can occur only at cost of reducing extent of moisture removed from the filter cake and vice versa → Not possible to improve two performance measures simultaneously

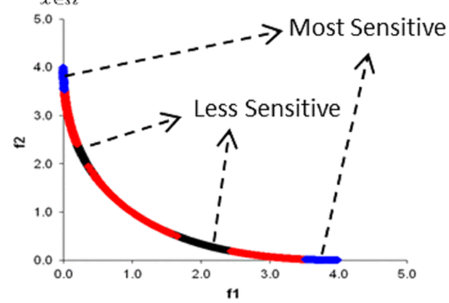
Sasanka Raha, Kartic C. Khilar, Pradip, and Prakash C. Kapur

New Decision Making Criterion for Multiobjective Optimization Problems

Ind. Eng. Chem. Res., 2018, 57 (3), 1014–1025
DOI: 10.1021/acs.iecr.7b04196

- Formulation of a polymer design
- discrimination among Pareto solutions set → selection of single alternative (the least sensitive one); real life example

$$\min_{x \in \Omega} F(x) = \{f_1(x) \cdots f_i(x) \cdots f_k(x)\}$$



Lívia Pereira Lemos , Enrique Luis Lima, and José Carlos Pinto

Multiobjective Optimization of Cyclic Adsorption Processes

Ind. Eng. Chem. Res., 2002, 41 (1), 93–104
DOI: 10.1021/ie010288g

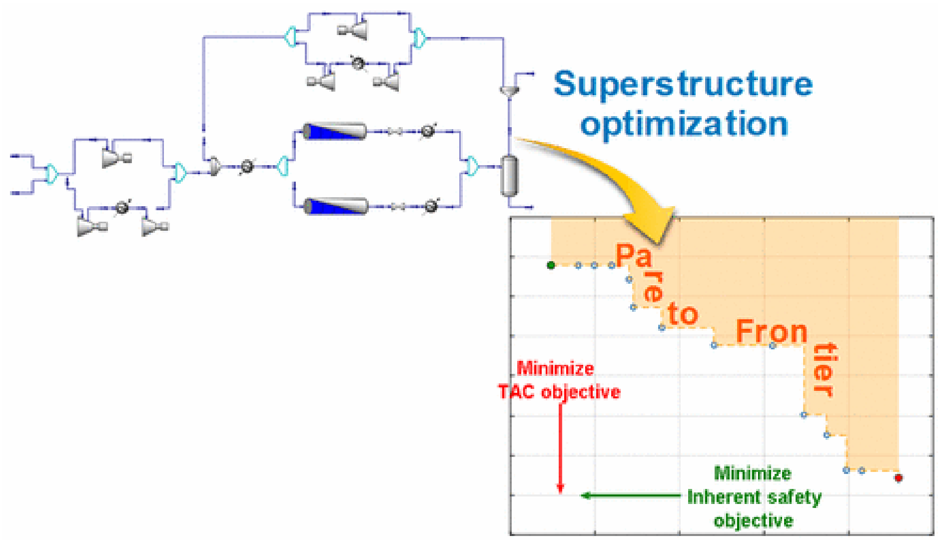
- multiobjective optimization programming→Single ObjFn(SWOF)
  - ® summation of a weighted objective function
    - Traditional ; simplest way
    - Remedy: Modified SWOF
      - approximates the Pareto curve efficiently

Daeho Ko, and Il Moon

Systematic Tools for the Conceptual Design of Inherently Safer Chemical Processes

Ind. Eng. Chem. Res., 2017, 56 (25), 7301–7313
DOI: 10.1021/acs.iecr.7b00901

- Task: [synergy of merging Process System Engineering tools with inherent safety principles]
- Design: superstructure that comprises several alternatives for streams, equipment, and process conditions
- ConflObject: [total annualized cost, Dow's Fire and Explosion Index]
- Method: Pareto set of solutions



Rubén Ruiz-Femenia , María. J. Fernández-Torres, Raquel Salcedo-Díaz, M. Francisca Gómez-Rico, and José A. Caballero

Efficient approach for calculating Pareto boundaries under uncertainties in chemical process design

Ind. Eng. Chem. Res., (2017)xxx,
DOI: 10.1021/acs.iecr.7b02539

- Task: [Distillation column]
- Design variables/Parameters : [Physical model parameters; Design parameters; Operating parameters; Evaluation parameters]
- uncertain Pareto boundaries
- uncertainties taken into account by worst and best case Pareto boundaries or by considering robustness of the Pareto boundary with respect to uncertain model parameters as additional objectives
- sensitivity analysis of Pareto boundary
- going beyond sensitivity analysis can yield favorable process designs not seen by sensitivity analysis alone
- adaptive scalarization approach

M. Bortz, J. Burger, E. v. Harbou, M. Klein, J. Schwientek, N. Asprion, R. Bottcher, K.-H. Kufer, and H. Hassez

Reactors

Multiobjective Optimization of a Fixed Bed Maleic Anhydride Reactor Using an Improved Biomimetic Adaptation of NSGA-II

Ind. Eng. Chem. Res., 2012, 51 (8), 3279–3294
DOI: 10.1021/ie202276q

- Process: Fixed bed maleic anhydride reactor
- ObjFns: [Single; Two, Multiple]
- ConflObject: [maximum productivity; minimum operating cost; minimum pollution]
- Alg.: [NSGA-II-Ajg]; [Alt-NSGA-II-Ajg] ;
- biomimicking the altruism of honeybees
  - converges to the optimal solutions faster than does NSGA-II-aJG
    - If #ObjFns =2
    - If #ObjFns =3, inferior solutions

Pranava Chaudhari and Santosh K. Gupta

Multiobjective Optimization of Unseeded and Seeded Batch Cooling Crystallization Processes

Ind. Eng. Chem. Res., 2017, 56 (20), 6012–6021
DOI: 10.1021/acs.iecr.7b00586

- Task1: unseeded batch cooling crystallization of paracetamol
- MultiObject: [Mean size ; coefficient of variation]
- Task: seeded batch cooling crystallization of potassium nitrate
- MultiObject: [mean size, CV, nucleated mass]
- Method: Pareto front

K. Hemalatha and K. Yamuna Rani

Distillation

Investigation of Separation Efficiency Indicator for the Optimization of the Acetone–Methanol Extractive Distillation with Water

Ind. Eng. Chem. Res., 2015, 54 (43), 10863–10875
DOI: 10.1021/acs.iecr.5b02015

- Nonsorted genetic algorithm (NSGA) →
- GA Paretofront further optimized focusing on decreasing energy cost by
  - sequential quadratic programming (SQP) →

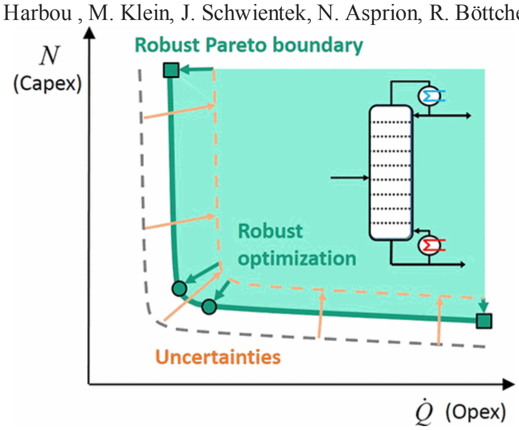
Xinqiang You, Ivonne Rodriguez-Donis, and Vincent Gerbaud

Efficient Approach for Calculating Pareto Boundaries under Uncertainties in Chemical Process Design

Ind. Eng. Chem. Res., 2017, 56 (44), 12672–12681
DOI: 10.1021/acs.iecr.7b02539

- Distillation column
- Adaptive scalarization : deals with uncertainties in multicriteria optimization

M. Bortz , J. Burger , E. von Harbou , M. Klein, J. Schwientek, N. Asprion, R. Böttcher, K.-H. Küfer, and H. Hasse



Multiobjective Optimization Approach for Integrating Design and Control in Multicomponent **Distillation** Sequences

Ind. Eng. Chem. Res., 2015, 54 (49), 12320–12330
DOI: 10.1021/acs.iecr.5b01611

- calculation of the condition number and the total annual cost of each design

José Antonio Vázquez-Castillo, Juan Gabriel Segovia-Hernández, and José María Ponce-Ortega

Multiobjective Optimization of a Hydrodesulfurization Process of Diesel Using Distillation with Side Reactor

Ind. Eng. Chem. Res., 2014, 53 (42), 16425–16435
DOI: 10.1021/ie501940v

- Task: hydrodesulfurization process
- Nonlinear-multivariable multiobjective optimization; continuous and discrete design variables
- Pareto solutions → opt conditions

Erick Yair Miranda-Galindo, Juan Gabriel Segovia-Hernández, Salvador Hernández, and Adrián Bonilla-Petriciolet

Procedure for the Selection among Technologies. Treatment of Deodorizer Distillate Oil

Ind. Eng. Chem. Res., 2014, 53 (43), 16803–16812
DOI: 10.1021/ie500211u

- Task: processing of deodorizer distillate oil
- ConflObject: [max(net present value) ; Min(generation of greenhouse gases measured as kilogram-equivalent of CO_2)
- Math.task: Multiobjective optimization mixed integer linear program

Daniela S. Laoretani and Oscar A. Iribarren

Reactive Thermally Coupled Distillation Sequences: Pareto Front

Ind. Eng. Chem. Res., 2011, 50 (2), 926–938
DOI: 10.1021/ie101290t

- Task: [optimal design of reactive complex distillation systems with thermal coupling for production of fatty esters]
- Task.Maths: nonlinear and multivariable problem; nonconvex with several local optimums and constraints; conflicting objectives

- traditional optimization methods
  - converge to local optimums
  - fail to capture the full Pareto optimal front
- Soln: multiobjective genetic algorithm with restrictions coupled to Aspen ONE Aspen Plus,
- previously used in the design and optimization of intensified distillation systems

Erick Yair Miranda-Galindo, Juan Gabriel Segovia-Hernández, Salvador Hernández, Claudia Gutiérrez-Antonio, and Abel Briones-Ramírez

Multiobjective Design of Reactive Distillation with Feasible Regions

Ind. Eng. Chem. Res., 2008, 47 (19), 7284–7293
DOI: 10.1021/ie800306b

- Task: [multiobjective design of complex reactive distillation columns]
- few heuristic rules about the distribution of the reaction

Rui M. Filipe, Scott Turnberg, Steinar Hauan, Henrique A. Matos and Augusto Q. Novais

Multiobjective Optimization of an Unseeded Batch Cooling Crystallizer for Shape and Size Manipulation

Ind. Eng. Chem. Res., 2015, 54 (7), 2156–2166
DOI: 10.1021/acs.iecr.5b00173

- ObjFns: [length mean size ; target aspect ratio (AR) of final crystals]

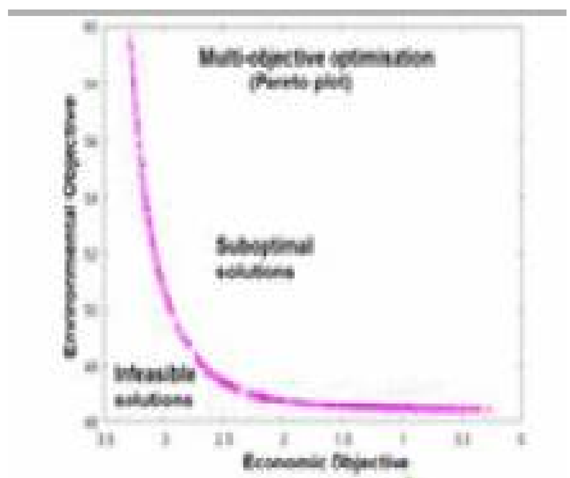
David Acevedo, Yanssen Tandy, and Zoltan K. Nagy

Life Cycle Optimization

Life Cycle Optimization for Sustainable Algal Biofuel Production Using Integrated Nutrient Recycling Technology

ACS Sustainable Chem. Eng., 2017, 5 (11), 9869–9880
DOI: 10.1021/acssuschemeng.7b01833

- Task: design of the algal biofuel production system
- ConflObject: [Gross annual profitability (economic) ; global warming potential (environmental criteria)]



Muhammadu Bello, Panneerselvam Ranganathan , and Feargal Brennan

Life Cycle Optimization of Biomass-to-Liquid Supply Chains with Distributed–Centralized Processing Networks

Ind. Eng. Chem. Res., 2011, 50 (17), 10102–10127
DOI: 10.1021/ie200850t

- Task: [optimal design and planning of biomass-to-liquids (BTL) supply chains under economic and environmental criteria]
- supply chain: [multisite distributed–centralized processing networks for biomass conversion and liquid transportation fuel production]
- Case Study: [county-level Ex. Iowa state]
- Objective.economic: [total annualized cost]; Objective. environPerformance: [life cycle greenhouse gas emissions]
- Model: [multiobjective, multiperiod, mixed-integer linear programming] ; ModelComponents: [diverse conversion pathways and technologies, feedstock seasonality, geographical diversity, biomass degradation, infrastructure compatibility, demand distribution, government incentives]
- Model: bicriterion opt; Method.: Pareto-optimal curve; Method.Soln.Pareto: ε-constraint
- Pred.Simultaneous: [optimal network design, facility location, technology selection, capital investment, production planning, inventory control, and logistics management decisions]

Fengqi You and Belinda Wang

Biomass and biofuels; Life cycle optimization; MINLP; Sustainable supply chain

Ind. Eng. Chem. Res., 2010, 49 (6), pp 2841–2848
DOI: 10.1021/ie901685m

- Task: [design of a chemical process for effectively adjusting calorific values in an offshore regasification terminal]
- design : [one objective generalized disjunctive programming (GDP) task ; multiobjective problem for min([operating costs; performance of natural gas liquids]).
- GDP (mathematically mapped into) →[mixed-integer nonlinear programming (MINLP)]
- MINLP technique incorporated into the process simulator
- Solution of resulting bicriterion problem with MINLP,: [heuristic procedure that reduces the number of discrete solutions which are necessary for complete Pareto optimal sets]

Hosoo Kim, Ik Hyun Kim and En Sup Yoon

Separation of racemic mixtures

Design and Performance Assessment of Continuous Crystallization Processes Resolving Racemic Conglomerates

Cryst. Growth Des., 2018, 18 (3), 1686–1696
DOI: 10.1021/acs.cgd.7b01618

- separation of enantiomers forming conglomerates in the solid state
- attainable enantiomeric excess and productivity
- complete resolution of racemic feed mixtures of conglomerate forming substances

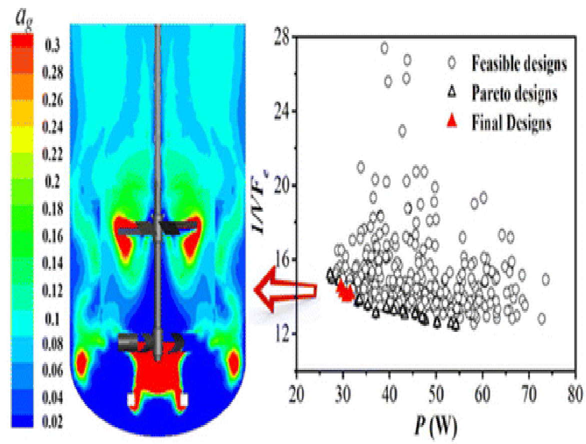
Till Köllges and Thomas Vetter

Computational Fluid Dynamics

Optimization of Dual-Impeller Configurations in a Gas–Liquid Stirred Tank Based on Computational Fluid Dynamics and Multiobjective Evolutionary Algorithm

Ind. Eng. Chem. Res., 2016, 55 (33), 9054–9063
DOI: 10.1021/acs.iecr.6b01660

- computational fluid dynamics (CFD) with multiobjective evolutionary algorithm (MOEA)
- maximize the overall effective gas holdup and minimize the power consumption with six geometrical variables. The nondominated sorting genetic algorithm-II (NSGA-II) was applied to construct a Pareto front



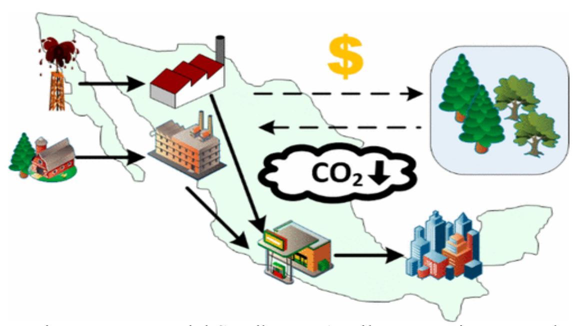
Miaona Chen, Jiajun Wang, Siwei Zhao, Chaozhong Xu, and Lianfang Feng

Physical Space

Environment

Optimal Design of Energy Systems Involving Pollution Trading through Forest Plantations

ACS Sustainable Chem. Eng., d 5 (3), 2585–2604
DOI: 10.1021/acssuschemeng.6b02928



Aurora de Fátima Sánchez-Bautista, José Ezequiel Santibañez-Aguilar, Fengqi You , and José María Ponce-Ortega

Environmental and Economic Optimization

Environmental and Economic Optimization of Algal Biofuel Supply Chain with Multiple Technological Pathways

Ind. Eng. Chem. Res., 2018, 57 (20), 6910–6925
DOI: 10.1021/acs.iecr.7b02956

- economic and environmental objectives: [Minimization of total supply chain cost; total life cycle greenhouse gas emission]
- multiobjective mixed integer linear programming approach
  - [multiple production pathways; time periods; seasonality factors; water evaporation; recycling opportunities; major traits of algal biofuel SCN]
- → optimal strategic and tactical level decisions of all SCN echelons.
- Pareto-optimal solutions: [fuzzy solution-based ε-constraint method] → [trade-off between economic and environmental objectives]
- Prediction: seven states of the U.S which intends to develop the algal biofuel SCN from the year 2018 to the year 2024
- Impact of future on present prediction: [Essential information with regard to the future of different technological pathways; relative importance of various supply chain factors; sensitivity analysis]

Keivan Ghasemi Nodooshan , Reinaldo J. Moraga , Shi-Jie Gary Chen , Christine Nguyen, Ziteng Wang, Shayan Mohseni

Groundwater

Optimal Design of a Rotating Packed Bed for VOC Stripping from Contaminated Groundwater

Ind. Eng. Chem. Res., 2012, 51 (2), 835–847
DOI: 10.1021/ie201218w

- volatile organic compounds (VOCs)
- ConflObject: [total annual cost ;total VOC removal]
- Method: Pareto-optimal solutions
- Scope: provides a wide range of optimized design alternatives

Krishna Gudena, G. P. Rangaiah, and S. Lakshminarayanan

Multiobjective Optimization of Cyclone Separators Using Genetic Algorithm

Ind. Eng. Chem. Res., 2000, 39 (11), 4272–4286
DOI: 10.1021/ie990741c

- Task: [industrial problem—treatment of 165 m3/s of air]
- ConflObject: [maximization (overall collection efficiency); minimization (pressure drop)]
- X: Decision variables: [number of cyclones; eight geometrical parameters of the cyclone]
- Nondominated Pareto optimal →
- optimal values (decision variables)
- Influencing factors: [diameters of the cyclone body; vortex finder, number of cyclones used in parallel]

G. Ravi, Santosh K. Gupta, and M. B. Ray

Supply Chains

Dynamic Operability Analysis of Process Supply Chains for Forest Industry Transformation

Ind. Eng. Chem. Res., 2014, 53 (23), 9825–9840
DOI: 10.1021/ie500608w

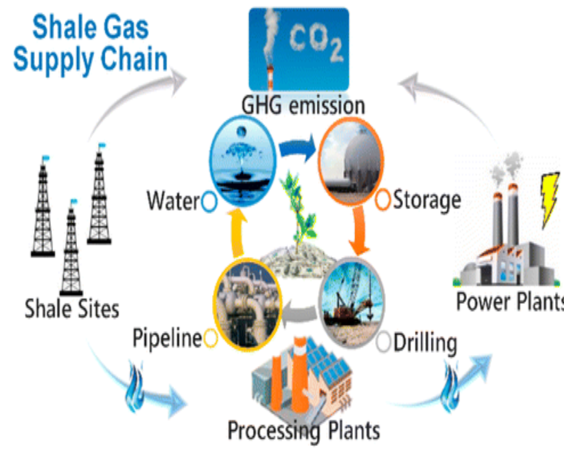
- ConflObject: [economics; response criterion]

Richard Mastragostino and Christopher L. E. Swartz

Shale Gas Supply Chain Design and Operations toward Better Economic and Life Cycle Environmental Performance: MINLP Model and Global Optimization Algorithm

ACS Sustainable Chem. Eng., 2015, 3 (7), 1282–1291
DOI: 10.1021/acssuschemeng.5b00122

- Task: cooperative shale gas supply chain →
- ConflObject: [economic; environmental] → opt trade-off by Pareto
- Method: multiobjective nonconvex mixed-integer nonlinear programming
- case study: Marcellus shale play
  - greenhouse gas emission of electricity generated from shale gas ranges from 433 to 499 kg CO2e/MWh,
  - levelized cost of electricity ranges from $69 to $91/MWh.



Jiyao Gao and Fengqi You

Multiobjective Optimization Using Goal Programming for Industrial Water Network Design

Ind. Eng. Chem. Res., 2014, 53 (45), 17722–17735
DOI: 10.1021/ie5025408

- Math.task: Mixed-integer linear programming
- case study: Industrial water network : [10 processes, 1 contaminant, and 1 water regeneration unit]
- real industrial case study: [12 processes, 1 contaminant, 4 water regeneration units addition of temperature requirements for each process]
- antagonist objectiveFns: [total freshwater flow rate; number of connections; total energy consumption]

Manuel A. Ramos, Marianne Boix, Ludovic Montastruc, and Serge Domenech

Design of Sustainable Product Systems and Supply Chains with Life Cycle Optimization Based on Functional Unit: General Modeling Framework, Mixed-Integer Nonlinear Programming Algorithms and Case Study on Hydrocarbon Biofuels

ACS Sustainable Chem. Eng., 2013, 1 (8), 1003–1014
DOI: 10.1021/sc400080x

- ObjectFns: [economics and environmental];
- Method : [Pareto-optimal frontier] ; Trade-off between Confl.Multiple.Objects
- mixed-integer linear fractional programming

Dajun Yue, Min Ah Kim, and Fengqi You

Identifying Key Life Cycle Assessment Metrics in the Multiobjective Design of Bioethanol Supply Chains Using a Rigorous Mixed-Integer Linear Programming Approach

Ind. Eng. Chem. Res., 2012, 51 (14), 5282–5291
DOI: 10.1021/ie2027074

- Task: Design of a bioethanol/sugar SC in Argentina
- MultiObjectFns: [five environmental goals]; Soln: [Pareto]
- Rigorous mixed-integer linear programming
- Basis: dimensionality reduction method which minimizes the error of omitting objectives

A. Kostin, G. Guillén-Gosálbez, F. D. Mele, and L. Jiménez

Single-Objective and Multiobjective Designs for Hydrogen Networks with Fuel Cells

Ind. Eng. Chem. Res., 2014, 53 (14), 6006–6020
DOI: 10.1021/ie404068p

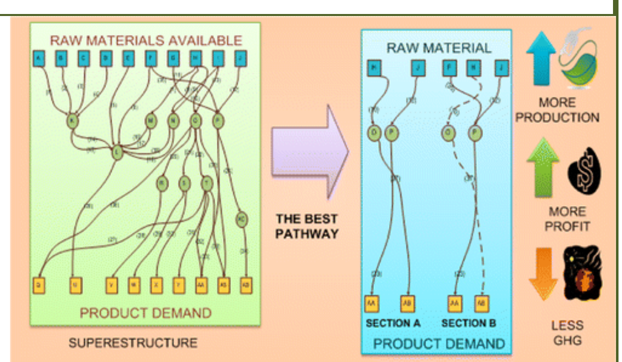
- ConflObject: [cost reduction ; pollution control (global CO_2 emission rate)]
- Meth: Pareto front

Yen-Cheng Chiang and Chuei-Tin Chang

Optimization of Pathways for Biorefineries Involving the Selection of Feedstocks, Products, and Processing Steps

Ind. Eng. Chem. Res., 2013, 52 (14), 5177–5190
DOI: 10.1021/ie303428v

- Task: [optimal selection of biorefinery configuration for conditions of Mexico under several scenarios]
- disjunctive programming model
- ConflObject: [max(net profit) ; min(greenhouse gas emissions)]
- Constraints: [number of processing steps]
- Method : [ε-constraint for Pareto curves]



Pascual Eduardo Murillo-Alvarado, José María Ponce-Ortega, Medardo Serna-González, Agustín Jaime Castro-Montoya, and Mahmoud M. El-Halwagi

Pareto Approach in Designing Optimal Semicontinuous Water Networks	Ind. Eng. Chem. Res., 2012, 51 (17), 6116–6136 DOI: 10.1021/ie2024728

- Case Study: semicontinuous water network (batch with respect to the raw materials)
- Task: [searching {particular successions of topologies; operating conditions}]
- Multi.lObjectFns: [min(freshwater consumption; investment ; operating costs]
- Method: [GA ; RK-type integrator]
- Software: Matlab built in functions

Elena-Lăcrămioara Dogaru and Vasile Lavric

A Multiobjective Optimization Approach for the Simultaneous Single Line Scheduling and Control of CSTRs	Ind. Eng. Chem. Res., 2012, 51 (17), 5881–5890 DOI: 10.1021/ie201740s

- Varibles: [integer, continuous]; process: [dynamic]
- Bicriterion Opt → mixed-integer dynamic optimization (MIDO) problem
- Paretofront-of-each-problem: ε-constraint method
- Multi.ObjFns casted into singleObjFn is inferior to multiobjective optimization techniques

Miguel Angel Gutiérrez-Limón, Antonio Flores-Tlacuahuac, and Ignacio E. Grossmann

Analysis of Carbon Policies in the Optimal Integration of Power Plants Involving Chemical Looping Combustion with Algal Cultivation Systems	ACS Sustainable Chem. Eng., 2018, 6 (4), 5248–5264 DOI: 10.1021/acssuschemeng.7b04903

- trade-offs between multiple objectives (economic and environmental) → different Pareto sets.

Aurora del Carmen Munguía-López, Vicente Rico-Ramírez , and José María Ponce-Ortega

Toward Economically and Environmentally Optimal Operations in Natural Gas Based Petrochemical Sites	Ind. Eng. Chem. Res., 2018, 57 (17), 5999–6012 DOI: 10.1021/acs.iecr.7b04598

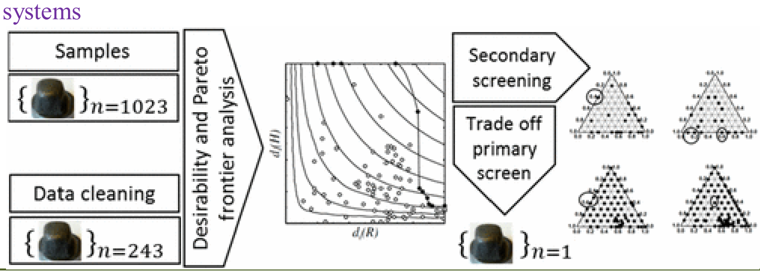
Task: Integrated petrochemical complex-sustainable operations

- Pareto-optimal curve →
- trade-off between the economic and environmental aspects

Antonio González-Castaño, J. Alberto Bandoni , and M. Soledad Diaz

Trade-Off Analysis in High-Throughput Materials Exploration	ACS Comb. Sci., 2017, 19 (3), 145–152 DOI: 10.1021/acscombsci.6b00122

- Task: optimum compositions in metal alloys with certain desired properties
- experimental data: from over 200 different compositions belonging to four different alloy systems



Kalpana K. Volety and Guido P. J. Huyberechts

Economic and Environmental Assessment of Alternatives to the Extraction of Acetic Acid from Water	Ind. Eng. Chem. Res., 2011, 50 (18), 10717–10729 DOI: 10.1021/ie201064x

- For each of alternatives, detailed optimization (ε-constraint method) was performed → Pareto's curves
- individual Pareto curves → compound Pareto's curve
- superimpose the individual Pareto'scurves for alternatives → to identify the trade-offs of this multiobjective optimization → best alternatives, optimum operational conditions.

Norberto García and José A. Caballero

Selective Hydrogenation of Methylacetylene and Propadiene in an Industrial Process: A Multiobjective Optimization Approach	Ind. Eng. Chem. Res., 2011, 50 (3), 1453–1459 DOI: 10.1021/ie100994j

- Task: [industrial selective hydrogenation process for methylacetylene and propadiene]
- Optimum operating conditions: Multiple-conflicting objective optimization with constraints
- Method: fuzzy-based membership function for Pareto-optimal solution
- → desired operating conditions like ratios of H2 to MAPD at each reactor and the recycle ratio

Wei Wu and Yu-Lu Li

Optimal Planning of a Biomass Conversion System Considering Economic and Environmental Aspects	Ind. Eng. Chem. Res., 2011, 50 (14), 8558–8570 DOI: 10.1021/ie102195g

- Task: [planning production of a biorefinery in Mexico]
- ObjectFn.Economic: [availability of bioresources, processing limits, demand of products, costs of feedstocks, products, processing routes]
- . ObjFn.EnvImpact : [overall environmental impact measured through the eco-indicator-99 based on the life cycle analysis methodology)]
- ConflObject: [Max(profit) ; Min(environmental impact)]

José Ezequiel Santibañez-Aguilar , J. Betzabe González-Campos, José María Ponce-Ortega , Medardo Serna-González , and Mahmoud M. El-Halwagi

Multi-Objective Lot-Sizing and Scheduling Dealing with Perishability Issues	Ind. Eng. Chem. Res., 2011, 50 (6), 3371–3381 DOI: 10.1021/ie101645h

- Task : [Diary company producing yogurt]
- MultiObjectFns: [multi-objective lot-sizing ; scheduling model]
- Soln.Method: [NSGA-II] → decision maker can arrive at true choice between different trade-offs from the Pareto front

Pedro Amorim, Carlos H. Antunes, and Bernardo Almada-Lobo

Resiliency Issues in Integration of Scheduling and Control	Ind. Eng. Chem. Res., 2010, 49 (1), 222–235 DOI: 10.1021/ie900380s

- Different layers of hierarchy in optimization and control → Integration of scheduling and control in process manufacturing systems
- Model: deterministic integrated scheduling and control [Flores-Tlacuahuac, A.; Grossmann, I. E. Ind. Eng. Chem. Res. 2006, 45, 6698]
- Robust integration of the scheduling and control layers in an uncertainty analysis framework → yields robust manufacturing systems
  - + performs well in the presence of the parametric variations.
- Uncertainty analysis: [chance constrained program; fuzzy; robust opt.]
- Multiobjective Pareto: [takes care of impact of the uncertainty on the different manufacturing objectives]

Kishalay Mitra, Ravindra D. Gudi, Sachin C. Patwardhan and Gautam Sardar

Optimization of Recovery Processes for Multiple Economic and Environmental Objectives	Ind. Eng. Chem. Res., 2009, 48 (16), 7662–7681 DOI: 10.1021/ie802006w

- Method: [elitist NSGA]
- Pareto-optimal Soln
    - elucidate the trade-offs present
    - decision maker's preference has to be declared
    - decision maker would be better equipped in choosing the best solution
    - identifies the best Pareto-optimal solution

- two case studies
- sustainability: [economic development, environmental stewardship, and societal equity]

economic criteria: [profit before taxes, payback period, net present worth] --well established,

- environmental impacts:[impact on humans, ecosystem—terrestrial and aquatic, and local/global temperatures—global warming and ozone depletion, as well as photochemical oxidation, acid rain, and eutrophication]

Elaine Su-Qin Lee and G. P. Rangaiah

Stochastic Combinatorial Optimization Approach to Biopharmaceutical Portfolio Management	Ind. Eng. Chem. Res., 2008, 47 (22), 8762–8774 DOI: 10.1021/ie8003144

- Task: [portfolio of five therapeutic antibody projects]
- MultiObjectFns: [maximizing profitability ; maximizing the probability of being profitable]
- Method: Pareto optimal front
- cluster analysis: identifies prevalence of broad and superior building blocks along the Pareto front.
- Key strategic decisions in biopharmaceutical portfolio management: [drug selection, activity scheduling, and third party involvement]

– Complications in optimizing strategies: [uncertainty, dependency relationships between decisions, multiple conflict objectives]

- Remedy: [stochastic combinatorial multiobjective optimization framework]
    + designed to address complications
    + framework simulates portfolio management strategies
    + harnesses Bayesian networks and evolutionary computation concertedly
    + characterizes probabilistic structure of superior decisions
    + evolves strategies to multiobjective optimality

Edmund D. George and Suzanne S. Farid

Optimal Operating Conditions of Microwave−Convective Drying of a Porous Medium	Ind. Eng. Chem. Res., 2008, 47 (1), 133–144 DOI: 10.1021/ie070738q

- Task: [to dry a porous medium via combined convective–microwave supplies]
- Design of experiments (DOE) & Response surface methodology
  - X: [drying time, maximum of overpressure in the material, energy balances of the process, material]
  - effects of drying parameters: [initial moisture, microwave power, air temperature, velocity, humidity) → → optimal operating (response surfaces)

Patrick Salagnac, Patrick Dutournié, and Patrick Glouannec

Pareto Optimal Solutions Visualization Techniques for Multiobjective Design and Upgrade of Instrumentation Networks	Ind. Eng. Chem. Res., 2003, 42 (21), 5195–5203 DOI: 10.1021/ie020865g

- Task: [design and upgrade of sensor networks:]
- visualization of Pareto optimal solutions (VisPOSs)
  1) projections of the POS onto specific two-dimensional surfaces
  2) representation of the problem in parallel coordinates systems

Miguel Bagajewicz, and Enmanuel Cabrera

Dynamic Model of an Industrial Steam Reformer and Its Use for Multiobjective Optimization	Ind. Eng. Chem. Res., 2003, 42 (17), 4028–4042 DOI: 10.1021/ie0209576

- MultiObjectFns: [min(cumulative (integrated over time) deviation of the flow rate of hydrogen);
  min(cumulative deviation of the steam flow rate)]
- Method : [elitist NSGA-II]

Anjana D. Nandasana, Ajay K. Ray, and Santosh K. Gupta

Application of Multiobjective Optimization in the Design and Operation of Reactive SMB and Its Experimental Verification	Ind. Eng. Chem. Res., 2003, 42 (26), 6823–6831 DOI: 10.1021/ie030387p

- Task: [design of reactive SMB processes]
- Method : [AI-based NSGA]

Weifang Yu, K. Hidajat, and Ajay K. Ray

Scheduling of Actual Size Refinery Processes Considering Environmental Impacts with Multiobjective Optimization	Ind. Eng. Chem. Res., 2002, 41 (19), 4794–4806 DOI: 10.1021/ie010813b

- Task: [scheduling problem of actual size refinery processes]
- ConflObject: [maximize (total profit) ; minimize (environmental impacts)]
- Plotting Pareto optimal solutions
  - decision makers pinpoint correlation between two objectives .
- Selection of one of Pareto optimal solutions
  - depends largely on the decision makers
- Model: [mixed-integer linear programming model]; Soln. : [ε-constraint method]

Jehoon Song, Hyungjin Park, Dong-Yup Lee, and Sunwon Park

Optimization of Venturi Scrubbers Using Genetic Algorithm	Ind. Eng. Chem. Res., 2002, 41 (12), 2988–3002 DOI: 10.1021/ie010531b

- Task: [pilot-scale scrubber]
- ConflObject: [maximization (overall collection efficiency) ; minimization (pressure drop)]
- X : [liquid–gas flow ratio, gas velocity in the throat ,aspect ratio]
- Soln: nondominated Pareto sets → Optimal design curves

G. Ravi, Santosh K. Gupta, S. Viswanathan, and M. B. Ray

Simulation and Multiobjective Optimization of an Industrial Hydrogen Plant Based on Refinery Off-Gas	Ind. Eng. Chem. Res., 2002, 41 (9), 2248–2261 DOI: 10.1021/ie010277n

- ConflObject: [maximization (product hydrogen and export steam rates) ;minimization(heat duty supplied to the steam reformer)]
- NSGA → Pareto-optimal operating conditions

P. P. Oh, G. P. Rangaiah, and Ajay K. Ray

Multiobjective Optimization of Steam Reformer Performance Using Genetic Algorithm	Ind. Eng. Chem. Res., 2000, 39 (3), 706–717 DOI: 10.1021/ie9905409

- ConflObject: [minimization (methane feed rate) ; maximization(flow rate of carbon monoxide in the syngas)]
- Soln.: Pareto-optimal operating conditions

J. K. Rajesh, Santosh K. Gupta, G. P. Rangaiah, and Ajay K. Ray

ACS.org; Sci.direct.com (SD): Information Source (is)

Data → Information → Knowledge → Intelligence

<I Kid>

Artificial Intelligence (AI) → Computational AI → Abstract AI → →

Brain → Mind → Consciousness →→ .....→

Super/hyper/beyond Intelligence .....

Object Oriented Terminology & (Geometric) Information (OOTI)

Multi-Object-Functions (MOF)

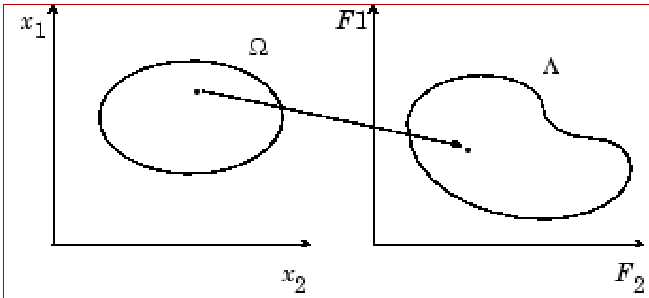
Dara → Fn → ObjFn → many (multi-) ObjFns → Soln(s) →

Pareto front → Performance measures → Set of Pareto solns →

Single_Pareto_Soln →

Knowledge Exploration

Data space to solution space			
Space.Math	**Pre-processing**	**Tasks**	**Solution characteristics**
🕮 Variables [X,y] 🕮 Parameters [Free; $$:distribution [normal; ..]] 🕮 functions 🕮 object functions 🕮 Solution	🕮 Raw 🕮 Scaled 🕮 Transformed [log; exp; [Fourier,...] 🕮 Projected [orthogonal [PCA, PLS,....],	🕮 Design 🕮 Solution	🕮 Valid/[feasible; infeasible] 🕮 Invalid



Mapping from variable space to object function space

Variable	:	[X,y]
X	:	[Explanatory; independent; design]
y	:	[Response; dependent;]

Functions (Fns) & Objective Fns (ObjFns)

Fn	:	[algebraic; trigonometric; ….., symbolic]
Fn(.)	:	Function(X or y)

ObjFn	:	[Fn([X, y] or Fn(X), or Fn(y)]
MulObjFns	:	[ObjFn1, ObjFn2, …. ObjFnj],

Constraints	:	[Equality, Inequality]
Constr.ineq	:	[< ; >; <++; >=]
Constr.eq	:	[=]

Multiple object functions with constraints

$$\min_{x \in \Omega} F(x) = \{f_1(x) \cdots f_i(x) \cdots f_k(x)\}$$
$$\text{subject to } g_i(x) \leq 0, i = 1, \ldots, m_1$$
$$h_j(x) = 0, j = 1, \ldots, m_2$$

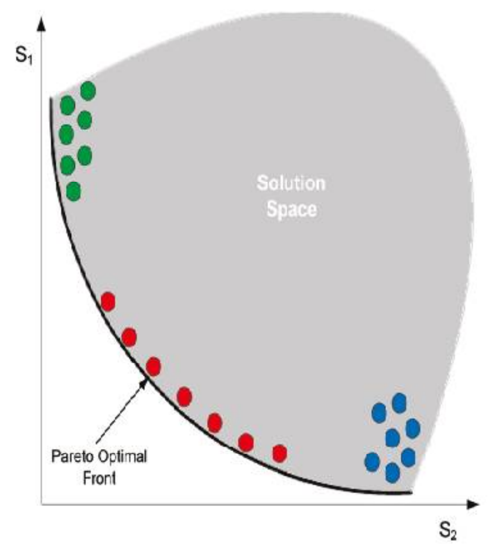
Knowledge bits (KB). ObJFns

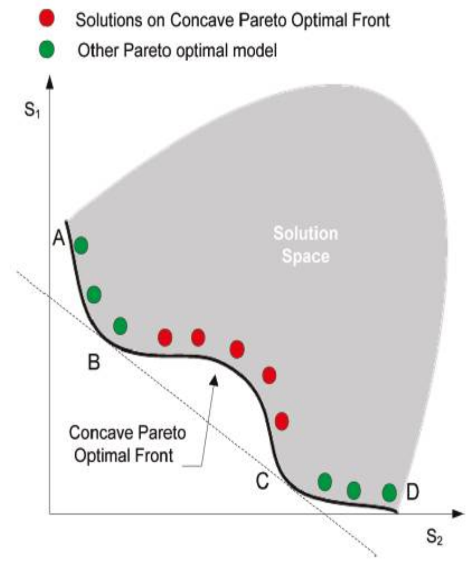
If NObjFns =1
Then Single object Function [SObjFn OR 1ObjFn;]

If NObjFns >1
Then MultiObjFns: [2ObjFns; 3ObjFns; many[4,5,….]ObjFns]

If NObjFns = 2
Then biObjFn [2ObjFns]

If NObjFns > 3
Then ManyObjFns [NObjFns = 4 OR 5 OR 6,….]





If	Non convexity in object functions and/or
	Non-convexity in feasible solution region
Then	nonconvex Pareto optimal front

Courtesy of J. Chem. Inf. Model. 2011, 51, 1656–1666

If	nonconvex Pareto optimal front
Then	weighted-sum approach will fail to find some Pareto optimal solutions

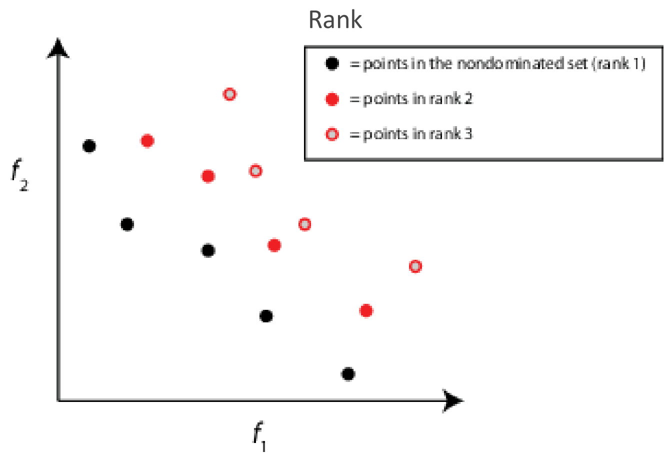
Goals and sub-goals

Goals	Sub-goals	→ Outcome →	
Model	Curve fitting	Solutions	Inferences
Control	Parametrization	Statistics	Knowledge bits
Prediction	Design		

Optimization of Objective Function(s) (Opt.ObjFns) → Solution Set(s)

Optimization	[unconstrained; constrained]
constrained	[Equality [=]; inequality [< OR >]]

SubGoal. ObjFn	:	min Or max (ObjFnj)
SubGoal. ObjFns.Conflict	:	[Min(ObjFnj) and Max(ObjFnk)]



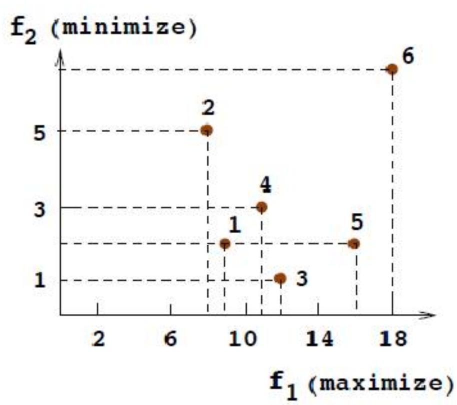
Rule →	**rank k individuals are dominated only by individuals in rank k - 1 or lower**
If	Rank 1 individuals
Then	They are not dominated by any other individuals
If	Rank 2 individuals
Then	They are dominated only by rank 1 individuals
KB:	All infeasible individuals have a worse rank than any feasible individual
If	Within the
Then	Rank-of-infeasible-population is the order by sorted infeasibility measure + highest rank for feasible members
If	Individuals are of lower rank
Then	They have a higher chance of selection
KB:	lower rank is better

Pareto Optimal Solutions (POS)

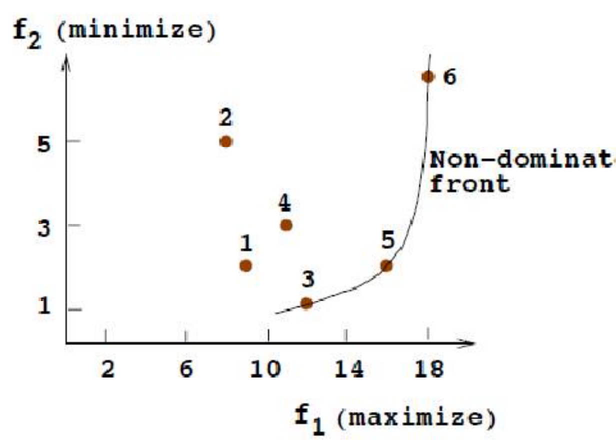
Nondominated set

P: A set of points;

Q: The set of points in P that are not dominated by any point in P

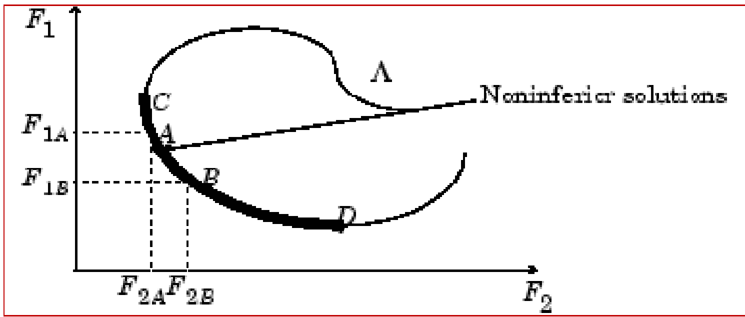


Conflicting bi-objFns



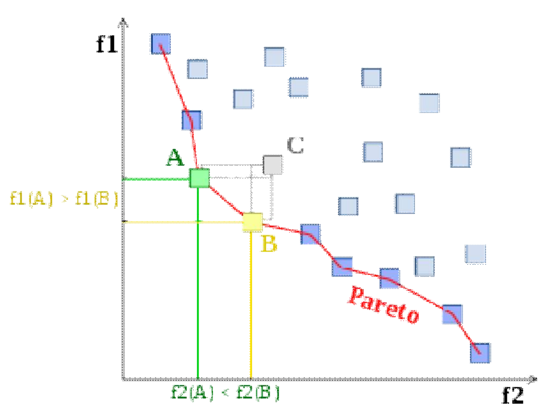
Non-dominant Pareto front

Non-inferior solution	Ω : set of solutions $x^* \in \Omega$ is a noninferior solution, if an improvement in one objective, F_1, requires a degradation in the other objective, F_2, i.e., $F_{1B} < F_{1A}$, $F_{2B} > F_{2A}$ i.e. if for some neighborhood of x^* there does not exist a Δx such that $(x^*+\Delta x)\in\Omega$ and $F_i(x^*+\Delta x)\le F_i(x^*)$, $i=1,\dots,m$, and $F_j(x^*+\Delta x)<F_j(x^*)$ for at least one j.



A and B : set of noninferior solutions lies on the curve in between C and D

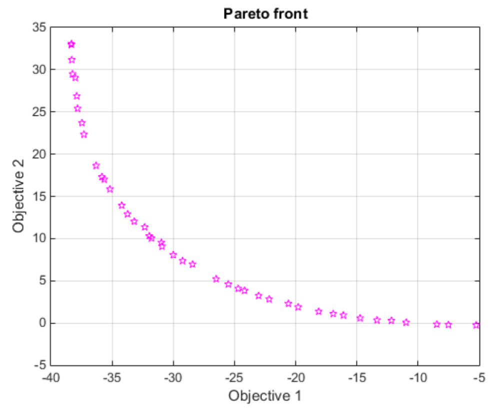
Pareto optimality	a tradeoff among conflicted objectives
Pareto optimal solution set	Solutions which are not dominated by any other Solutions in Solution set Any improvement in one objective of a Pareto optimal point must lead to deteriorations in at least one other objective. + deeper insights into the trade-off among the objectives and many choices for implementation
Pareto solution set	set of all the Pareto optimal points
Pareto optimal front	set of all the Pareto optimal objective vectors



Pareto front

boxed points	feasible solutions
KB	smaller values are preferred to larger ones
Because	Point C is not on the Pareto frontier it is dominated by both point A and point B.
So,	Points A and B are not strictly dominated by any other, do lie on the frontier

Courtesy of IEEE TRANS. EVOLUT. COMPUT, 6, (2) (2002) 182



- Objective function (F(1) and f(2)) space;
- Plot shows tradeoff between the two objectives

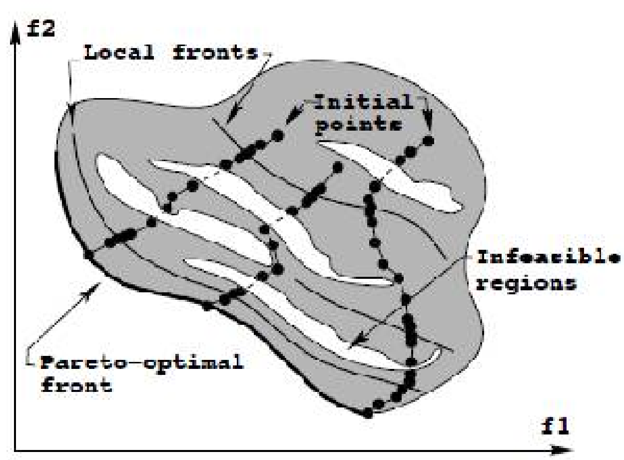
MatLab notation

```
f(1) = x(1)^4 - 10*x(1)^2+x(1)*x(2) + x(2)^4 -
(x(1)^2)*(x(2)^2);
f(2) = x(2)^4 - (x(1)^2)*(x(2)^2) + x(1)^4 +
x(1)*x(2);
```

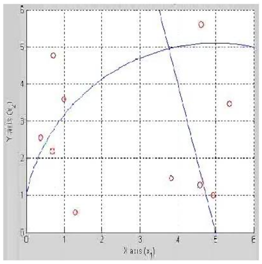
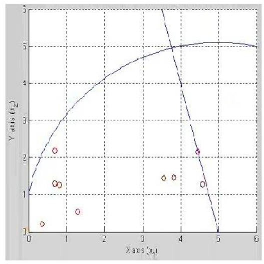
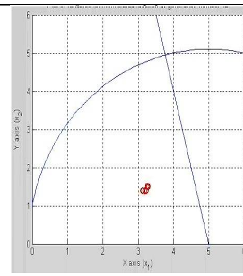
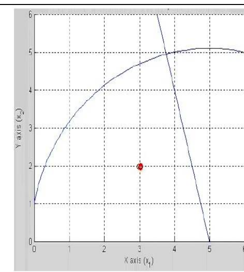
Xdim	[2; 60]	
Lower	[-5;-5]	
upper	[5;5]	
Pareto Front population fraction	0.7	User chosen

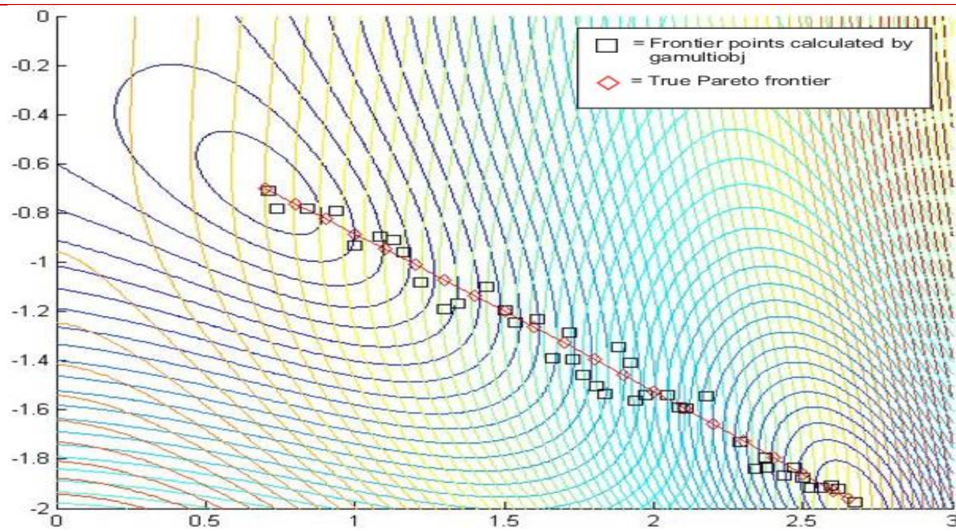
$$
\begin{aligned}
\text{Minimize} \quad & f(x) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2 \\
\text{subject to} \quad & g_1(x) \equiv 26 - (x_1 - 5)^2 - x_2^2 \geq 0, \\
& g_2(x) \equiv 20 - 4x_1 - x_2 \geq 0, \\
& 0 \leq (x_1, x_2) \leq 6.
\end{aligned}
$$

NP = 10;



Courtesy from K Deb report (2001)

			
Initial population	generation 5	generation 5	generation 100



- **2D-Contour of two objective functions;**
- **figure is in parameter space**;

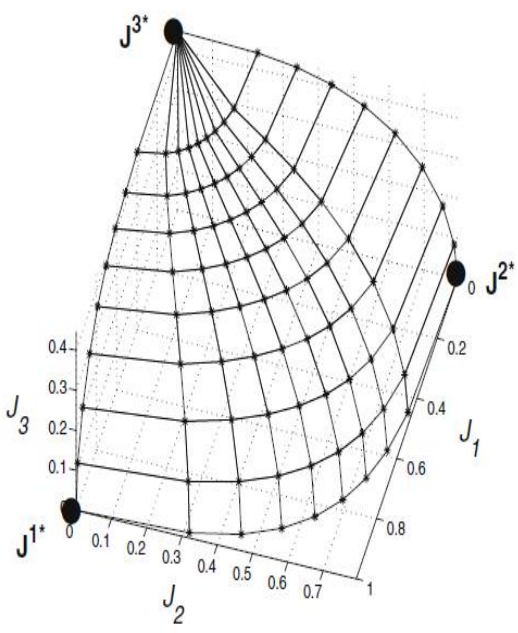
Methods for Calculation of Pareto Front

	A set of solutions is Pareto optimum
If	by moving from that solution to another in the feasible solution space, any improvement in the value of one of the objective functions results in the deterioration of at least one of the remaining objective functions

Methods.appoximating.true PeratoFront:	**Decomposition-based.Method**
Pareto dominance-based ;	multi-objective evolutionary algorithms (MOEAs);
performance indicator-based ;	MOEA/D ; MOEA/D-DRA; MOEA/D-AWA
decomposition-based;	[augmented €-constraint method (AUGMECON);

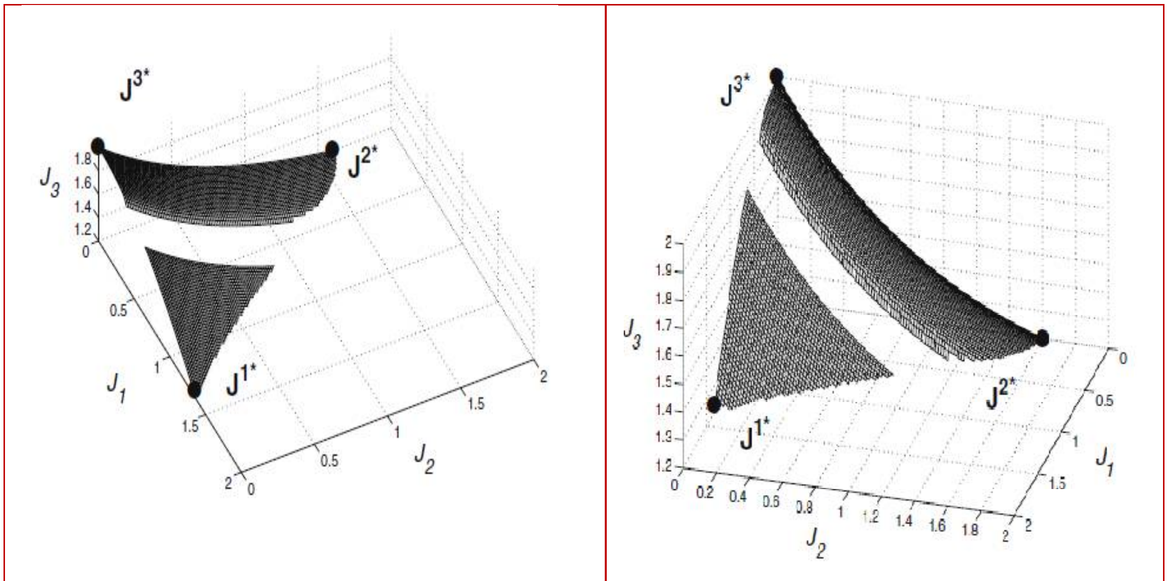
	AUGMECON2; 📖 simple augmented €-constraint method (SAUGMECON); 📖 decomposition based multi-objective evolutionary algorithm with the "-constraint framework (DMOEA-"C);
SMEA	Competitive multiobjective evolutionary algorithm. based on selforganizing mapping method (SOM) and neighborhood relationship concept.
MOCell	cellular-based and MO solver
SMPSO	PSO based multiobjective solvers

Pareto frontier generation algs.	[Constraint Proposal Method, Normal Constraint Method, Linear Weight Method]; [genetic alg; evolutionary alg.]
[GA; Evolv.A]	applied to solve complex multi-objective problems, + find solutions quickly ven in a complex solution space + a framework for effectively sampling large search spaces,



Pareto front by weighted sum method

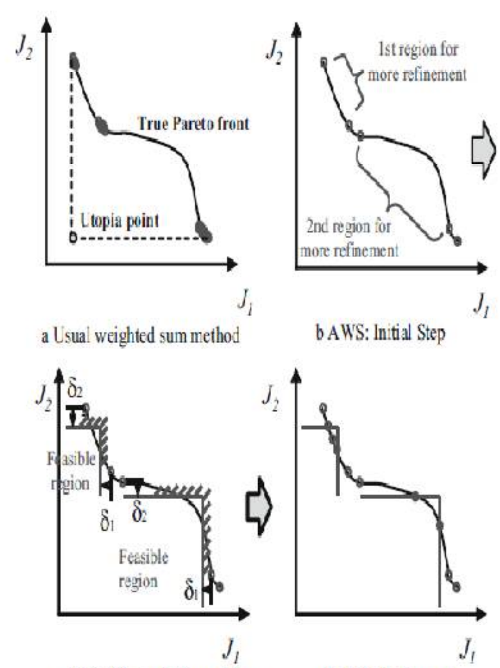
$$\begin{aligned} \text{maximize} \quad & [J_1 \; J_2 \; J_3]^T \\ \text{subject to} \quad & x_1^4 + 2x_2^3 + 5x_3^2 \le 1 \\ & J_1 = x_1 \\ & J_2 = x_2 \\ & J_3 = x_3 \\ & x_i \ge 0 \quad (i = 1, 2, 3). \end{aligned}$$



Two different perspective views of 3D-surface

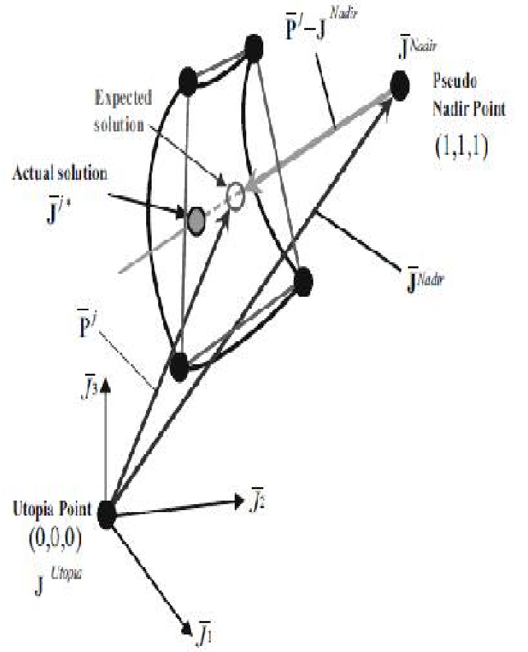
- overall surface of the Pareto front is nonconvex
  - middle front has nonconvex regions
    - disconnected due to dominated solutions region → looks like a valley

- boundary of Pareto front consists of three edge curves:
  - curve between J1∗ and J3∗ is convex with a gap due to a dominated solution region,
  - other two curves are not convex.



a Usual weighted sum method
b AWS: Initial Step
c AWS: Constraint imposition
d AWS: Refinement

Concept and procedure of the adaptive weighted sum (AWS) method



Configuration of an additional equality constraint for refinement

Performance measures in Pareto Front

- Inverted generational distance (IGD)
- Hyper volume (HV)
- additive€ -indicator ($I_{\epsilon+}$)

Choice of Single Pareto optimal solution

- gray relational analysis.
- simple additive weighting

Data → Information → Knowledge → Intelligence

<Diki>

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