Multicriteria Optimization and Decision Analysis (MODA)

Lecturer: Dr. Hao Wang

Master CS, 6 ECT

14x1.5h Lectures, incl. 2 Exercise Lectures
(all material & announcements on Brightspace)

Introduction - Organizational

- Dr. Hao Wang
  - h.wang@liacs.leidenuniv.nl
  - Room 272, Oort building
  - Another office t.b.d. in the new Gorlaeus building
  - Office hours: every Friday, 9 – 11, room 272, Oort building
- Contact email: moda.ta2024@gmail.com (for all questions and communications)

Introduction - Grading

- Exam (80%)

- Practical Assignments (20%):
  - Assignment 1 (10%): theoretical foundations
  - Assignment 2 (10%): algorithmics
  - Individual work
  - Deadline t.b.a.
- Final grade: 0.1 Grade Homework1 + 0.1 Homework2 + 0.8 Exam
- Pass: Final grade >= 5.5

- If your final score is 5 - 6, it will be rounded to 6.

- Otherwise, it will be rounded to the nearest 0.5. For example, if it is 6.2, you will get 6; if it is 6.25, you will get 6.5.

Learning goals – Introduction Unit

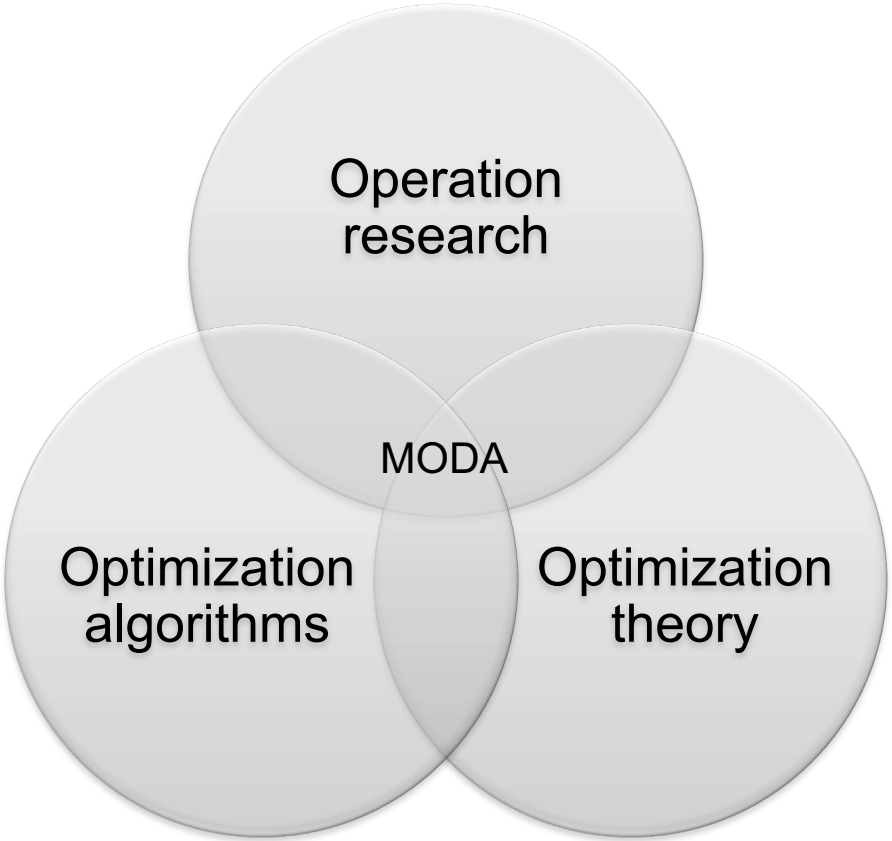
I. What is multicriteria optimization and decision analysis?

II. Structure of the course & requirements

III. How has this field developed? What were the major historical steps?

IV. Examples of multicriteria optimization problems. What are the criteria, search space, and constraints?

Class Contents



Class Contents

1. Linear and Nonlinear Programming
2. Multicriteria Decision Analysis
3. Order Theory and Pareto Dominance
4. Optimality Conditions in Multiobjective and Constrained Optimization (KKT Theorem)
5. Scalarization Methods and Single-Point Methods
6. Computational Complexity and Optimal Distributions
7. Meta-Heuristics and Evolutionary Methods
8. Case Studies & Exercises

Literature:

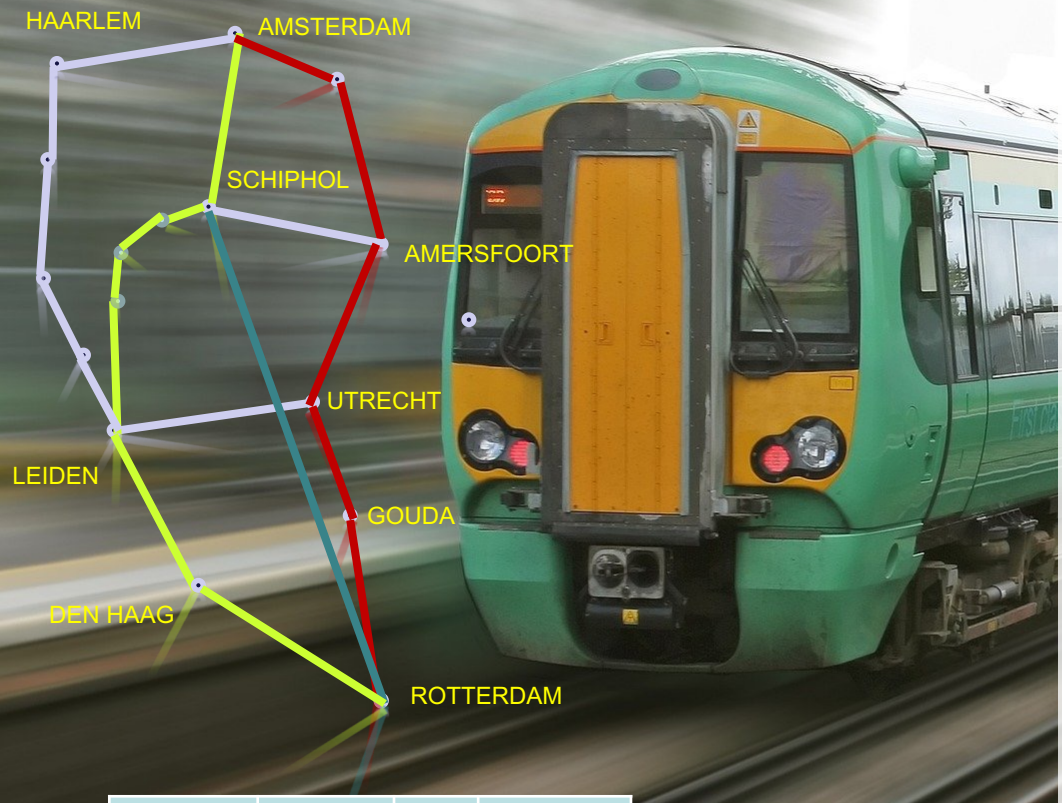
Emmerich, Michael, and André Deutz. "*Multicriteria optimization and decision making*." LIACS. Leiden university, NL (2017).

Slides, Exercises & Solutions

Tentative Schedule

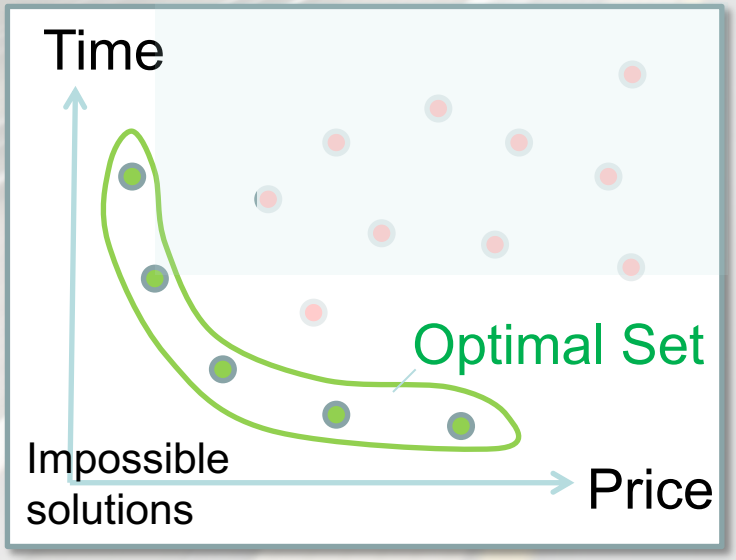
- Feb. 15: Intro. + Mathematical programming
- Feb. 22: Mathematical programming + Optimization complexity
- Feb. 29: Orders, Pareto dominance, and optimization
- March 7: Optimality conditions
- March 14: Optimality conditions exercises
- March 21: Single-point search algorithms
- March 28: Evolutionary/population-based algorithms
- April 4: Local optimization method + Set-oriented methods
- April 11: Set-oriented methods
- April 18: Exercises on algorithms
- April 25: Multicriteria Decision Analysis
- May 2: Advanced topics, e.g., optimal μ-distribution
- May 16: Advanced topics, e.g., Maximal Set algorithm
- May 23: Q&A

TOPIC OF MODA



Example 1: Alternative routes

- Time — Min
- Comfort — Max
- Price — Min



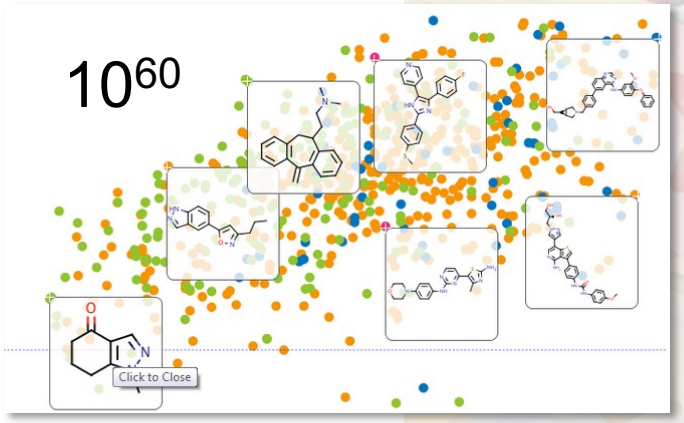
TICKET	T	C	P
OPT1	3:00 H	2	60 EUR
OPT2	3:00 H	1	65 EUR
OPT3	3:30 H	3	44 EUR
OPT4	4:30 H	2	41 EUR
OPT5	15:30	4	35 EUR
OPT6	15:34	4	32 EUR

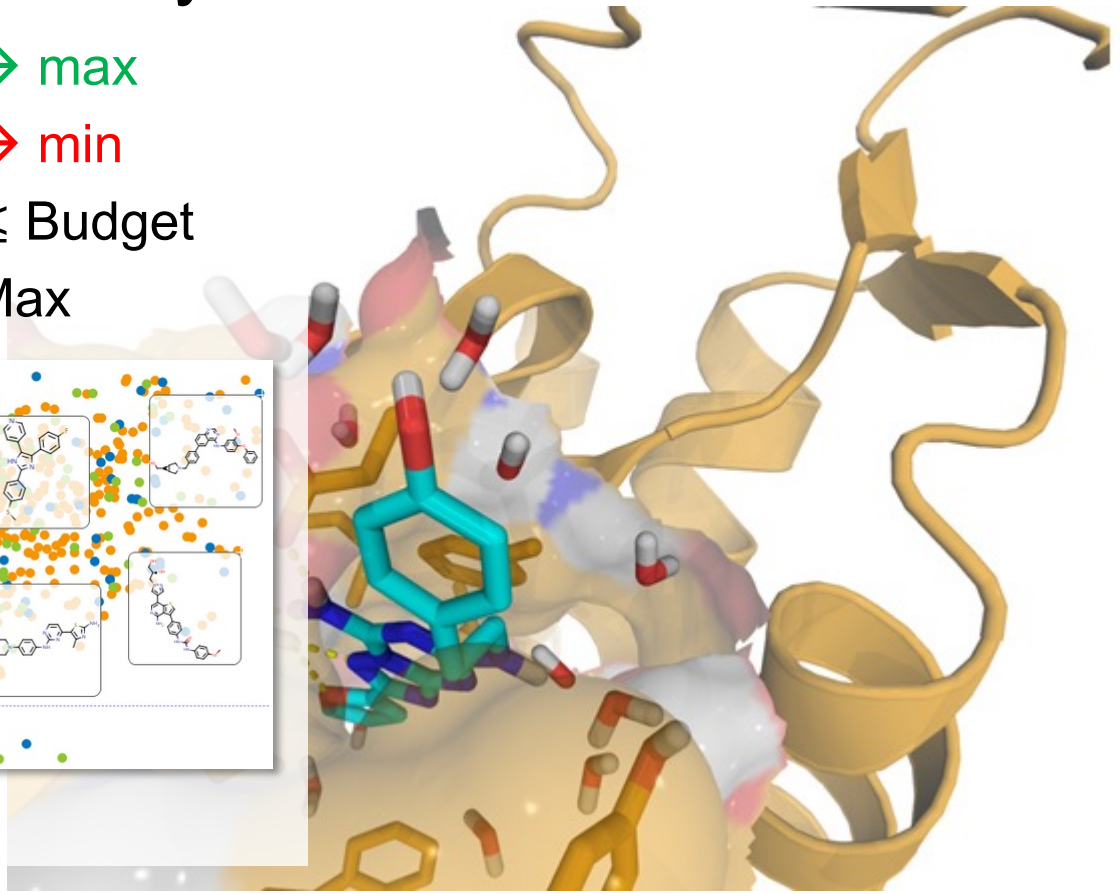
O(N!) different paths from Amsterdam to Rotterdam

https://pixabay.com/users/shutterbug75-2077322/

Example 2: *In-Silico* Drug Discovery

Activity	→ max
Side-effects	→ min
Cost	≤ Budget
Diversity	Max





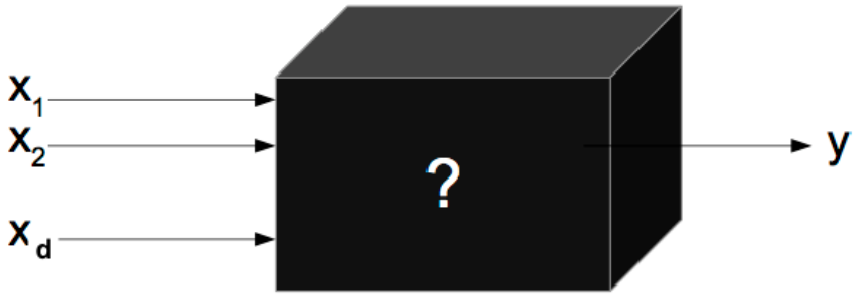
Picture: Universiteit Leiden, Data-Driven Drug Discovery Network (D4N) - Leiden University

Topics

- *(1) Problems and problem formulation*
  - White-box: Linear, nonlinear, quadratic…
  - Black-box
  - White/black-box constraints

$$\min_{\vec{x}\in\mathbb{R}^d} \vec{a}\cdot\vec{x}, \quad \text{s.t. } B\vec{x}-\vec{c}\geq 0$$

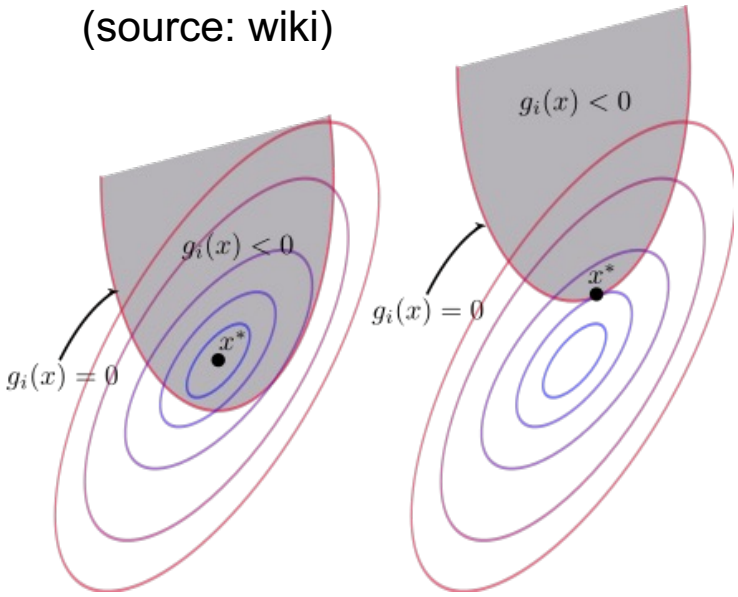
$$B\in\mathbb{R}^{n\times d}, \quad B_{ij}=b_{i,j}$$



Topics

- *(2) Optimality conditions*
  - Single-objective, multi-objective
  - First-order, second-order, *Karush-Kuhn-Tucker (KKT)*, Fritz John

Illustration of KKT
(source: wiki)



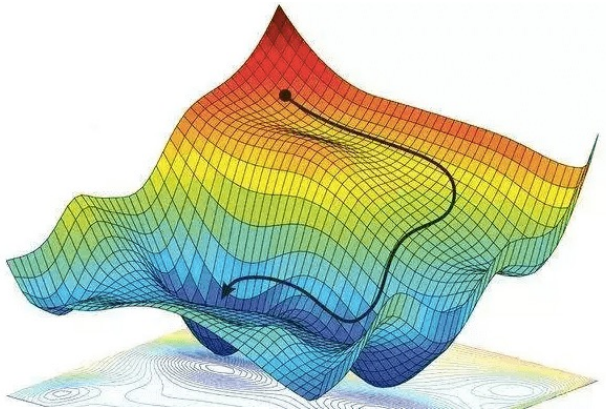
First-order condition:

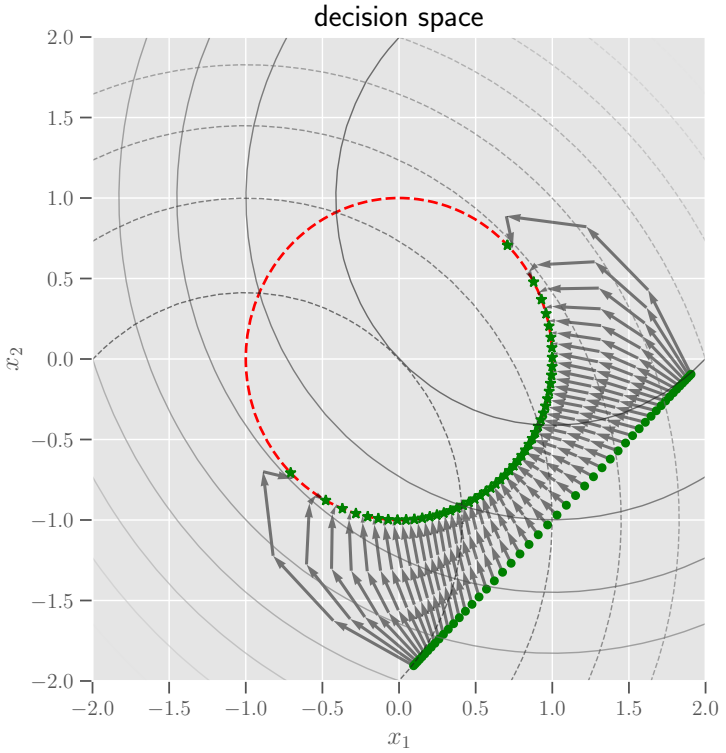
$$f \in C^\infty(\mathbb{R}^d)$$

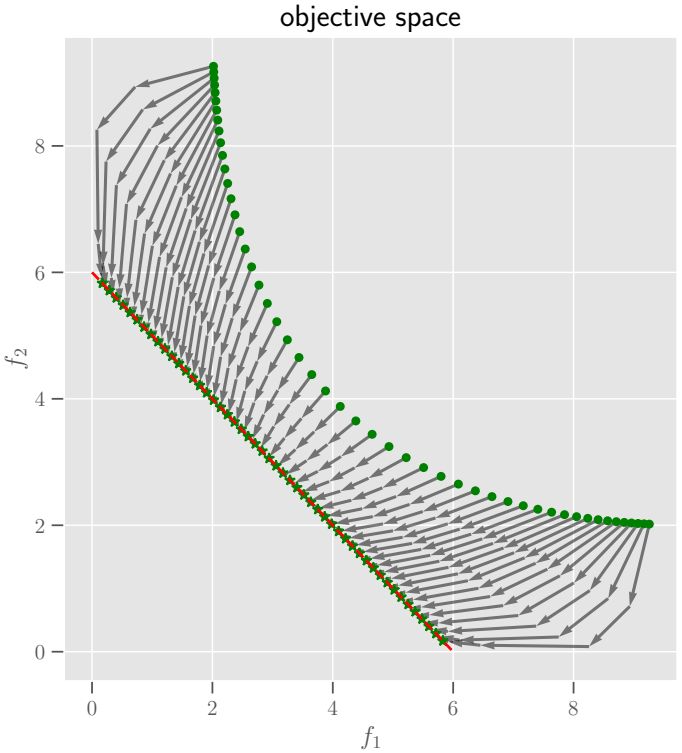
$$\{\vec{x} \in \mathbb{R}^d : \nabla f(\vec{x}) = 0\}$$

Topics

- *(3) Algorithms*
  - Direct/zero-order, single-point, population-based
  - Mathematical optimization methods: gradient, Newton

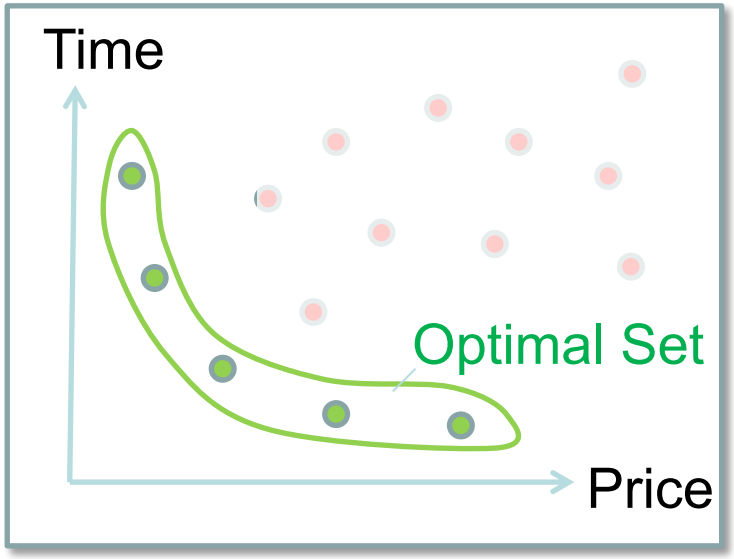






Topics

- *(4) Decision-making/analysis*
  - Which solution among the optimal set thereof should you choose?
  - How to take users' preference into account?



Multiobjective Mathematical Program

Let $x_1, \ldots, x_d$ denote d, $c_1, \ldots, c_n$, and $b_1, \ldots, b_q$ be defined as previous. A multiobjective mathematical programming problem (MOP) has the form:

$$\begin{aligned} f_1(x_1, \ldots, x_d) &\rightarrow \min \\ &\vdots \\ f_m(x_1, \ldots, x_d) &\rightarrow \min \end{aligned}$$

subject to

$$\begin{aligned} g_1(x_1, \ldots, x_d) &\geq c_1 \\ &\vdots \\ g_n(x_1, \ldots, x_d) &\geq c_n \\ h_1(x_1, \ldots, x_d) &= b_1 \\ &\vdots \\ h_q(x_1, \ldots, x_d) &= b_q \end{aligned}$$

For $m > 1$ one can always add the term 'Multiobjective', e.g. Multiobjective LP, Multiobjective MIP, etc..

Multicriteria Optimization and Decision Analysis

- Definition: *Multicriteria Decision Analysis (MCDA)* is a scientific field that studies evaluation of a finite number of alternatives based on multiple criteria. It provides systematic methods to compare, evaluate, and rank solutions.

- Definition: *Multicriteria Optimization* (MCO) is a scientific field that studies search for optimal solutions given multiple criteria and constraints. Here, usually, the search space is very large and not all solutions can be inspected (e.g., scheduling, design, control)

- Definition: *Multiobjective Decision Making* (MCDM) deals with MCDA and MCO or combinations of these.

- We use here the title: "***Multicriteria Optimization and Decision Analysis = MODA***" instead of MCDM in order to focus more on the algorithmically challenging optimization/operational research aspect.

Multi-parametric Complexity in Multicriteria Decision Analysis

- Number of variables/search space size n
- Number of objective functions m
- Number of constraint functions r
- Number of retrieved alternative solutions s
- Number of decision makers d
- Degree of (non-)linearity l (linear, quadratic, etc.)

$\Rightarrow$ Multi-parametric problem complexity $\Theta(n, m, r, s, d, l)$

HISTORICAL REMARKS

Early roots of MCDA

- A very early reference relating to Multiple Criteria Decision Analysis algorithms can be traced to Benjamin Franklin* (1706 1790)
- He allegedly had a simple paper system for deciding important issues.
  - Take a sheet of paper.
  - On one side, write the arguments in favor of a decision;
  - on the other side, write the arguments against.
  - Strike out arguments on each side of the paper that are relatively of equal importance.
  - When all the arguments on one side are struck out, the side which has the remaining arguments is the side of the argument that should be supported.

  Supposedly Franklin used this in making important decisions.

Source: http://www.mcdmsociety.org/facts.html

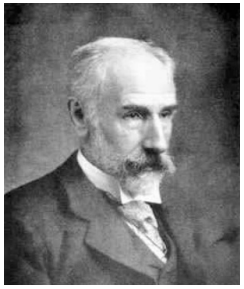
*Benjamin Franklin, polymath and founding father of USA 1706 – 1790

Development

- Vilfredo Pareto (1848–1923), an Italian economist who used the concept of Pareto efficiency in his studies of economic efficiency and income distribution:
- At the same time Francis Edgeworth defined ‘indifference curves’, the ‘core’ of an exchange economy, and the so-called ‘Edgeworth box’ based on a concept of local Pareto optimality for two criteria.
- When Kuhn and Tucker formulated optimality conditions for nonlinear optimization with constraints in 1951, they also considered problems with multiple objectives.

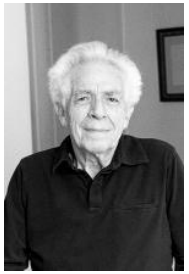
Vilfredo Pareto, Italian economist, 1848-1923

Francis Edgeworth, British Economist,

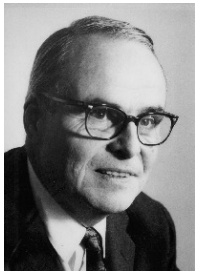


Around 1900

Harold W. Kuhn US-American Mathematician 1924-2014

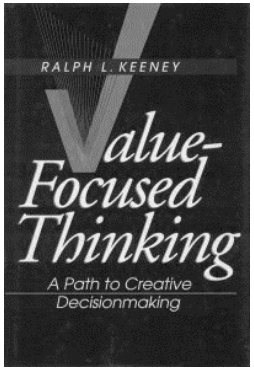


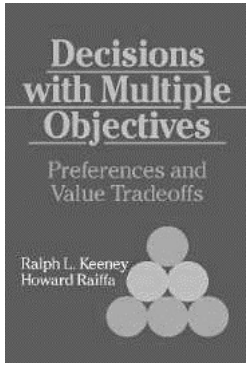
Albert William Tucker Canadian Mathematician, 1905-1995



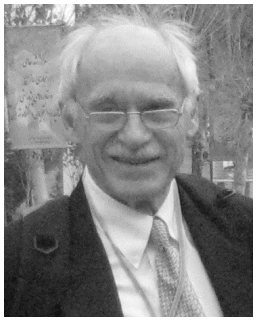
1951

https://www.princeton.edu/news/2014/07/05/harold-kuhn-princeton-mathematician-who-advanced-game-theory-dies-88?section=topstories





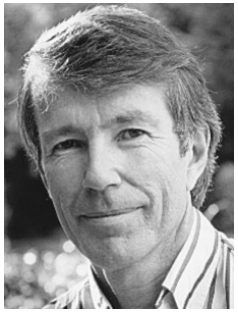
Development



Ralph Steuer,
US American Economist

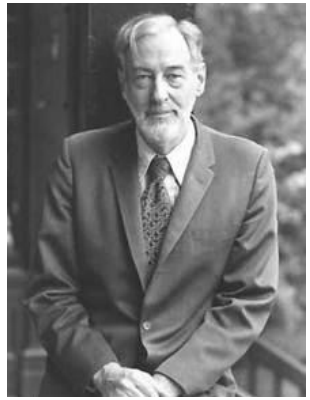
- Ralph Keeney and Howard Raiffa published an important work in 1976. This book was instrumental in establishing the theory of multiattribute value theory (including utility theory) as a discipline. It became a standard reference and text for many generations of study of decision analysis and MCDM.
- Ralph Steuer's professor, John Evans, suggested the topic of developing a multiple criteria simplex method to compute all efficient extreme points. Inspiration was drawn from earlier works of Karlin, Koopmans, and Geoffrion.

Howard Raiffa
*1924
US American
Economist



Ralph Keeney
US American
Decision Analyst

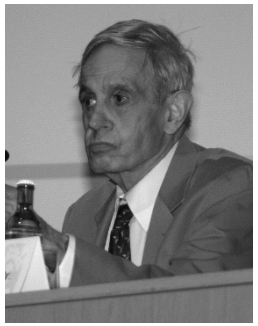
Tjalling Koopmans
1910-1985
Dutch
Mathematician
And Nobel Prize
(economics) winner



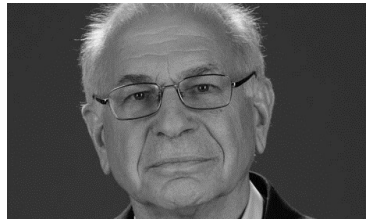
Development

- Kahnemann and Tversky studied the psychological aspects of decision making and pointed out (seemingly) irrational components in human decision making.
- In the closely related field of *game theory*, John von Neumann and later John Nash studied **decisions in games** with conflicting parties.
- Remark: Today, multiobjective game theory, is a topic at the intersection of MODA and game theory

John von Neuman, US -American Mathematican (1903-1957)



John Nash, US -American Mathematican (*1928) Nobel Price Economics



Daniel Kahneman (u,*1934-) & Amos Tversky (l,1937-1996), Israeli socio-psychologists, Nobel Price L

Source: wikipedia

Development

- Kaisa Miettinen published a book on Nonlinear Multiobjective Optimization (first edition 1999) which became a standard reference on deterministic methods for solving mathematical programming with multiple criteria.
- Kalyanmoy Deb published a seminal book on Evolutionary Multicriteria Optimization (EMO), including NSGA-II algorithm. The work on NSGA-II became the most cited computer science paper 2000-2010.
- Since then EMO is a very active field of research, not only in economics but also in (computer) science and engineering.
- Recently, new term “Many-objective optimization” for problems with >> 3 objectives, e.g. urban planning, multidisciplinary design.

Kaisa Miettinen,
Finnish Professor for Industrial Optimization
President of MCDM Society

Kalyanmoy Deb,
Indian Engineer & Computer Scientist
Endowed Koening Chair,
MSU Michigan

Recent advances: Lorentz Center Workshops: SIMCO 2013, SAMCO 2016, MACODA 2019

Indicator-based MCO
~ Using Statistical Progress Measures

Surrogate-Model Assisted MCO
~ Costly Evaluations (Simulators)

Take home messages

- The fields of **multicriteria decision analysis** and **multicriteria optimization** are distinguished by whether a small finite set is considered or search in a large search space.
- Multiple parameters influence the problem complexity
- The fields evolved in parallel, first in **economics/operations research** and later for other disciplines, especially **engineering**. and **data science**
- In machine learning goals are to minimize error rates (false positives, false negatives) & model complexity.
- In general, multicriteria optimization problems can be defined by the following components: **decision space**, **objectives**, **constraints**