Simulation-based optimization

Basic fundamentals and some examples

PennState

Modelling & Simulation Discussion Group
Wageningen University
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About Me

Waterschap De Dommel
Research stay (2015-2016)
UNIVERSITY OF LEICESTER
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Belarus
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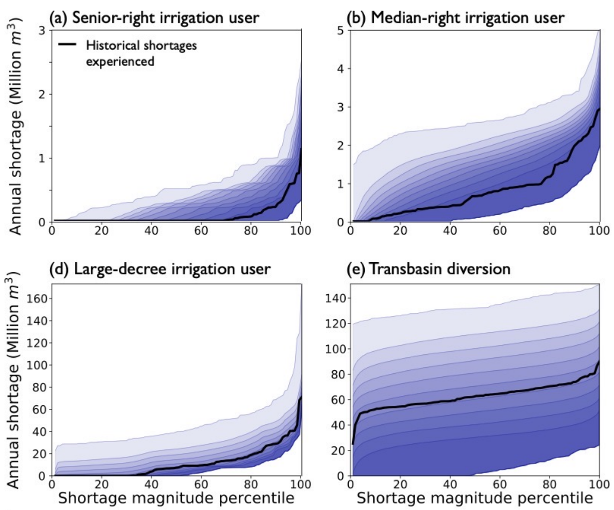
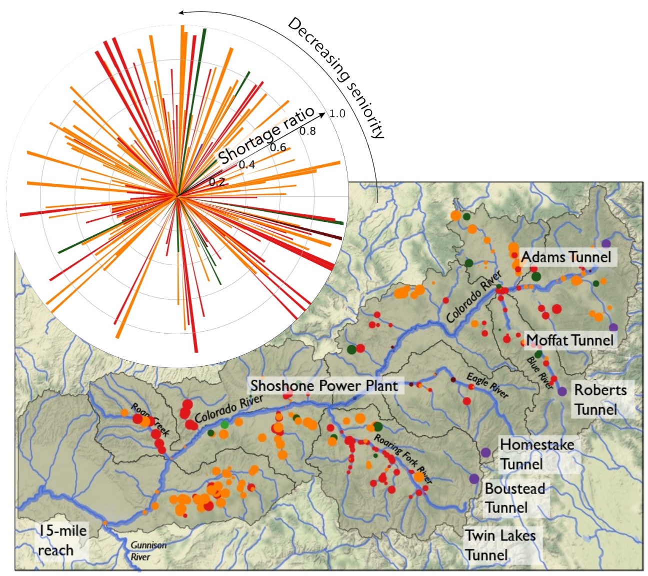
France
Romania
Italy
Spain
Portugal
Greece
Morocco
Algeria
Western Sahara
Mauritania
Mali
Niger
Chad
Sudan

Main Research Questions

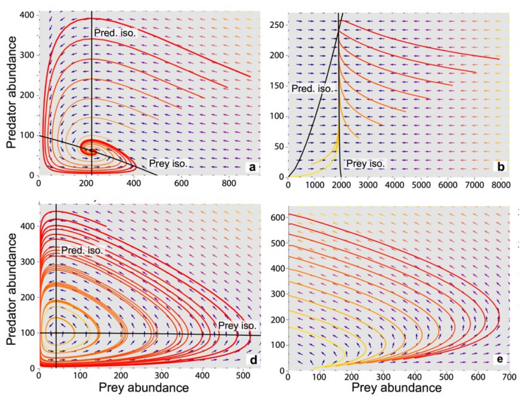
How is climate stress and other uncertainties affecting water resources and the people relying on them?



How are human systems interacting with each other and with environmental systems across scales?



What drives fundamental change in human-environmental systems?



Today's lecture

- How do we study systems?
- Why use simulations?
- Types of simulation approaches
- Basics of optimization
- Optimization for simple models
- Optimization for complex models

Ways to study a system

System

How would climate change affect this lake?
How would nearby development affect this lake?
How should we be managing/protecting this lake?
How can we know our actions will be effective?

Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

Ways to study a system

System

Experiment with actual system

Dove Lake, Australia

Alter the lake physically and see what happens

<u>Pros:</u>
Our findings are certainly valid

<u>Cons:</u>
Changes might be too expensive/disruptive/irreversible
Questions might be about the future

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Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

Ways to study a system

System

Experiment with actual system

Experiment with a model of a system

A 'surrogate' for the real system

<u>Pros:</u>

Cheaper, not affecting actual system

Allows us to ask future/hypothetical questions

<u>Cons:</u>

Imperfect representation of actual system

Are we modeling the right things?

Are we modeling things right?

Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

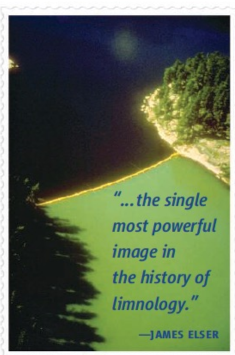
Ways to study a system


NEWSFOCUS

https://www.science.org/doi/10.1126/science.322.5906.1316

Canada's Experimental Lakes

In remote Ontario, a network of lakes is dedicated to bold ecological manipulations. Research there has helped explain algal blooms and acid rain. As the unique outdoor lab turns 40, some wonder whether it is past its prime



System

- Experiment with actual system
- Experiment with a model of a system
  - Physical model

Pros:
Closest analogs of real systems

Cons:
Impractical, costly, site availability

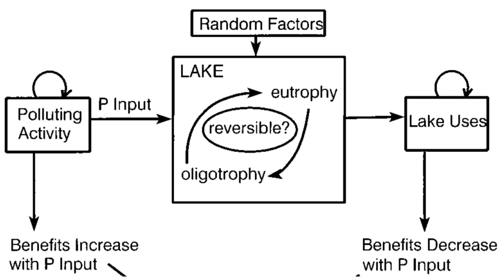
http://www.iisd.org/ela/

Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

Ways to study a system

System

- Experiment with actual system
- Experiment with a model of a system
  - Mathematical model
  - Physical model



$$\frac{dP}{dt} = l - sP + \frac{rP^q}{m^q + P^q}$$

How can we use this to answer the questions we are interested in?

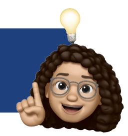
Carpenter et al. (1999) https://doi.org/10.1890/1051-0761(1999)009[0751:MOEFLS]2.0.CO;2

Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

Ways to study a system

System

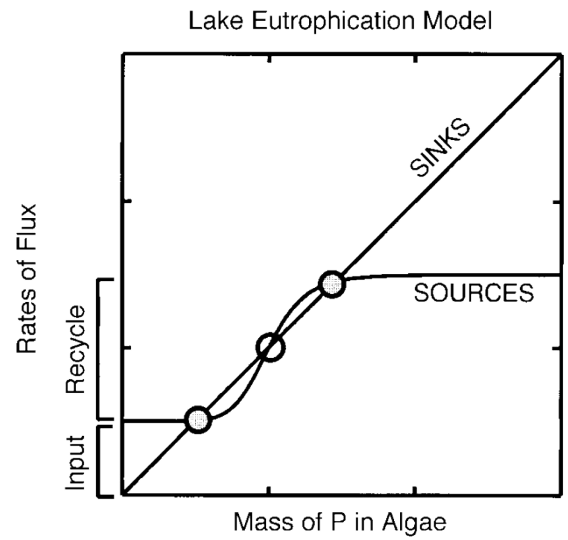
- Experiment with actual system
- Experiment with a model of a system
  - Mathematical model
    - Analytical solution
  - Physical model



Solve for different values to understand dynamics

$$\frac{dP}{dt} = l - sP + \frac{rP^q}{m^q + P^q}$$

Carpenter et al. (1999) https://doi.org/10.1890/1051-0761(1999)009[0751:MOEFLS]2.0.CO;2



Works best:
Simple models with tractable solutions

Struggles:
Complex systems with complex models

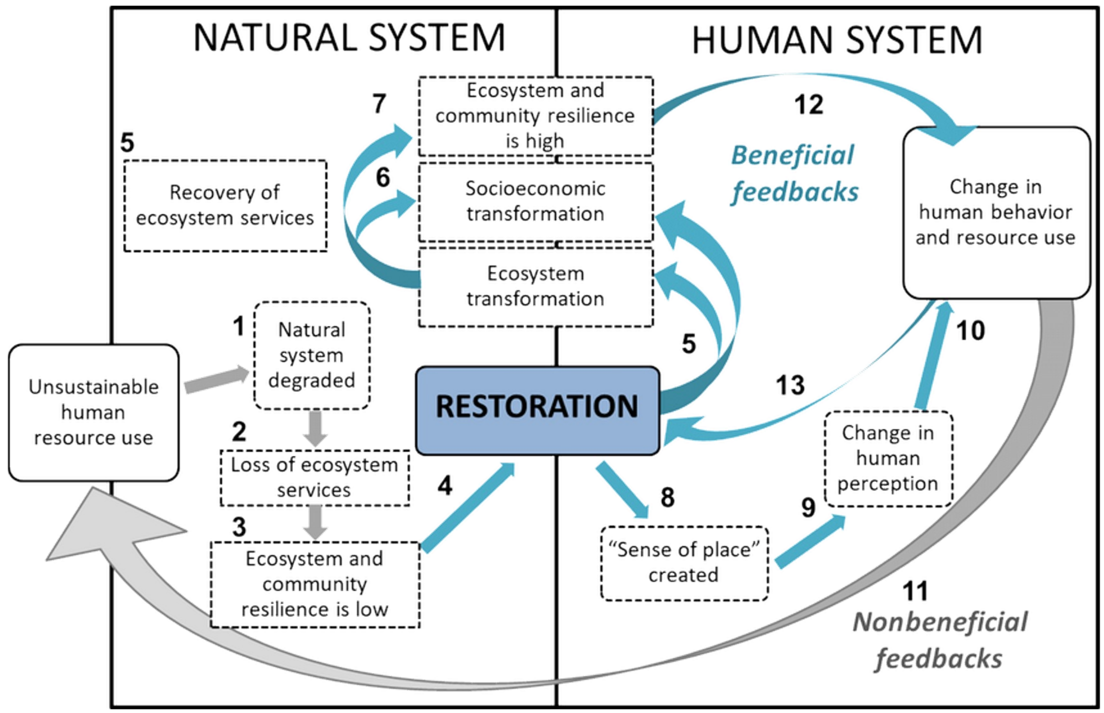
Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

Complex systems with complex models

Most systems have multiple interacting components

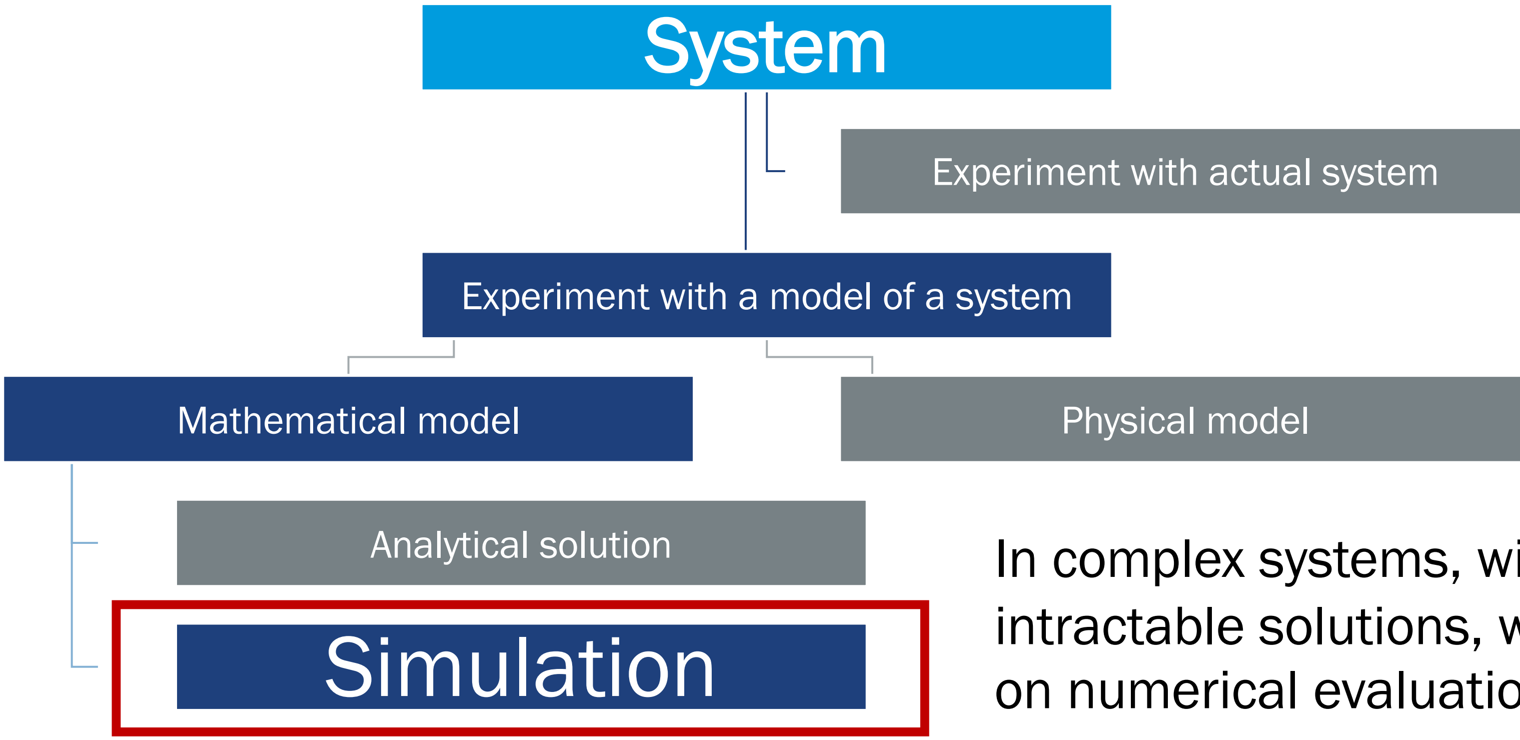
Each component may be modeled very differently, especially when humans are involved

Things get more complex when we are also looking at systems across scales



Kibler et al. (2018). https://doi.org/10.5751/ES-10542-230425

Ways to study a system



In complex systems, with intractable solutions, we rely on numerical evaluations

Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

Simulation is one of the most widely used techniques in scientific and industrial applications:

- Designing and analyzing manufacturing systems
- Evaluating logistics requirements and supply chains
- Designing and operating transportation systems such as airports, freeways, ports, and subways
- Evaluating designs for service organizations such as call centers, fast-food restaurants, hospitals, and post offices
- Understanding dynamics of physical, biological, environmental, and social systems
- Assessing alternative policies

Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

Types of simulation approaches

Static	Deterministic	Continuous
Dynamic	Stochastic	Discrete

Types of simulation approaches

Static

Dynamic

Deterministic

Continuous

Stochastic

Discrete

A static model is one which contains no internal history of either input values previously applied, values of internal variables, or output values.
An example is a function that maps an input variable to a dependent variable.

$$\begin{aligned} y_1 &= f_1(u_1, u_2, \ldots u_n,) \\ y_2 &= f_2(u_1, u_2, \ldots u_n,) \\ &\vdots \\ y_m &= f_m(u_1, u_2, \ldots u_n,) \end{aligned}$$

Examples: structural load, mechanical stress

Types of simulation approaches

Static

Dynamic

Deterministic

Continuous

Stochastic

Discrete

A dynamic model simulates the time-dependent behavior of systems, i.e., when a system evolves over time.

$$
\begin{aligned}
dx_1(t)/dt &= f_1(u_1(t), u_2(t), \ldots u_m(t),\ \ x_1(t), x_2(t), \ldots x_n(t)) \\
dx_2(t)/dt &= f_2(u_1(t), u_2(t), \ldots u_m(t),\ \ x_1(t), x_2(t), \ldots x_n(t)) \\
&\vdots \\
dx_n(t)/dt &= f_n(u_1(t), u_2(t), \ldots u_m(t),\ \ x_1(t), x_2(t), \ldots x_n(t))
\end{aligned}
$$

Examples: nutrient loading, atmospheric dynamics, traffic patterns

Types of simulation approaches

A deterministic model does not contain any probabilistic (i.e., random) components. Every model simulation always results in the same exact output.

Static

Deterministic

Continuous

Examples: chemical reactions, unit conversions, accounting calculations

Dynamic

Stochastic

Discrete

Types of simulation approaches

A stochastic model contains at least some probabilistic (i.e., random) components. Each model simulation might result in a different output.

Deterministic

Stochastic

Examples: bus schedules, market fluctuations, election results, weather

Types of simulation approaches

A **continuous model** is one for which the state variables change continuously with respect through time.

Examples: a plane flying through the sky, a tank filling with water

Static

Deterministic

Continuous

Dynamic

Stochastic

Discrete

Types of simulation approaches

Static

Deterministic

Continuous

A **discrete model** is one for which the state variables change instantaneously at separated points in time.

Dynamic

Stochastic

Examples: customers per day, switches between states "on/off"

Discrete

Types of simulation approaches

Few systems in practice are entirely discrete or entirely continuous, especially when looking at different scales.

Depending on the kind of change we're interested in, or the questions we are asking we can choose to model a system as either discrete or continuous.

Continuous

Discrete

Break for questions

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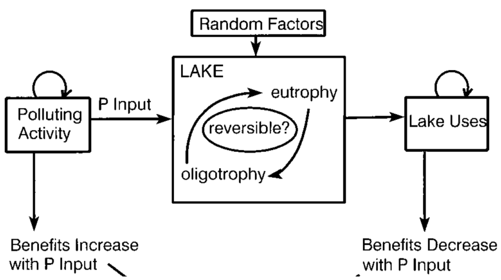
- Experiment with actual system
- Experiment with a model of a system
  - Mathematical model
  - Physical model



$$\frac{dP}{dt} = l - sP + \frac{rP^q}{m^q + P^q}$$

How can we use this to answer the questions we are interested in?

Carpenter et al. (1999) https://doi.org/10.1890/1051-0761(1999)009[0751:MOEFLS]2.0.CO;2

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Law, A. M.: Simulation modeling and analysis. McGraw-Hill, Boston, Mass., 2007.

Questions and model use

Descriptive – ***"What has happened/is happening?"***

Describe and interpret system behavior

Predictive – ***"What would happen if…?"***

Fill in missing information

Use established system relationships to predict new outcomes

Prescriptive – *"What should we do?"*

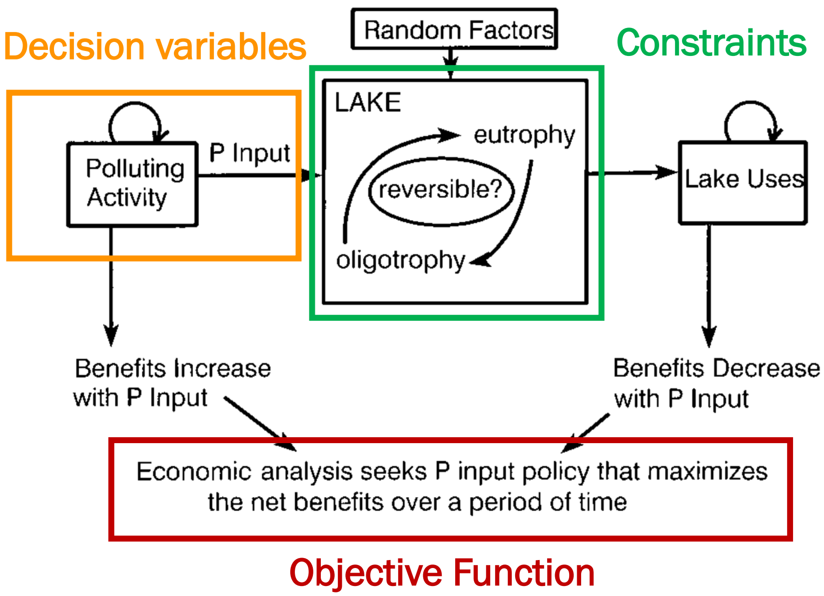
Independent variables are under control of decision maker

Model solutions tell the decision maker what actions to take

Focusing on objectives (goals) and constraints

- *If I want to achieve goal X, what should I do?*
- *What is the “best” action (or set of actions) to take?*
- *What are the limits of what we can achieve in this system?*
- *What are the tradeoffs across different system objectives?*

Basic terms of optimization problems



$$\frac{dP}{dt} = l - sP + \frac{rP^q}{m^q + P^q}$$

Decision variables: System components we can control (e.g., P_1, P_2, ..., P_n)

Objective Function: Describes our goal(s) for the system (e.g., Profit = 5 x P_1 + 10 x P_2)

Constraints: Restrictions on the system (e.g., $P_1 + 2 \times P_2 < 3$)

Carpenter et al. (1999) https://doi.org/10.1890/1051-0761(1999)009[0751:MOEFLS]2.0.CO;2

Let's demonstrate basic principles of optimization with a linear programming example

Betty owns a factory that produces leather and plastic suitcases at a cost of $50 each.

She earns $150 and $100 for each leather and plastic suitcase sold, respectively.

It takes Betty's factory 15 and 10 hours to make one leather and plastic suitcase respectively.

Betty has 1566 labor hours available.

Her factory only has 250 suitcase handles available. Leather suitcases need 1, plastic suitcases need 2.

What should Betty do to maximize her profits?

Linear programming example

0. Understand the problem

How many leather and plastic suitcases should Betty produce to get max profit?

1. Identify **variables** that can be changed (*decision variables*)

1. How many leather suitcases to make (X_1)
2. How many plastic suitcases to make (X_2)

2. Define **objective**

Maximize Profit = (\$150-\$50) X_1 + (\$100-\$50) X_2

3. Identify **constraints** that limit our choices (e.g. relationships among variables, non-negativity, etc.)

$15X_1+10X_2 \leq 1566$

$1X_1+2X_2 \leq 250$

$X_1, X_2 \geq 0$

Linear programming example

Maximize Profit: (\$150-\$50) X_1 + (\$100-\$50) X_2

Subject to:

$$15X_1+10X_2 \leq 1566$$
$$1X_1+2X_2 \leq 250$$
$$X_1, X_2 \geq 0$$

Any choice of values of (X_1, X_2) is called a **solution.**
A solution satisfying all the constraints is a **feasible solution.**
The set of all feasible solutions is called the **feasible region.**
A solution in the feasible region that maximizes the objective function is called an **optimal solution.**

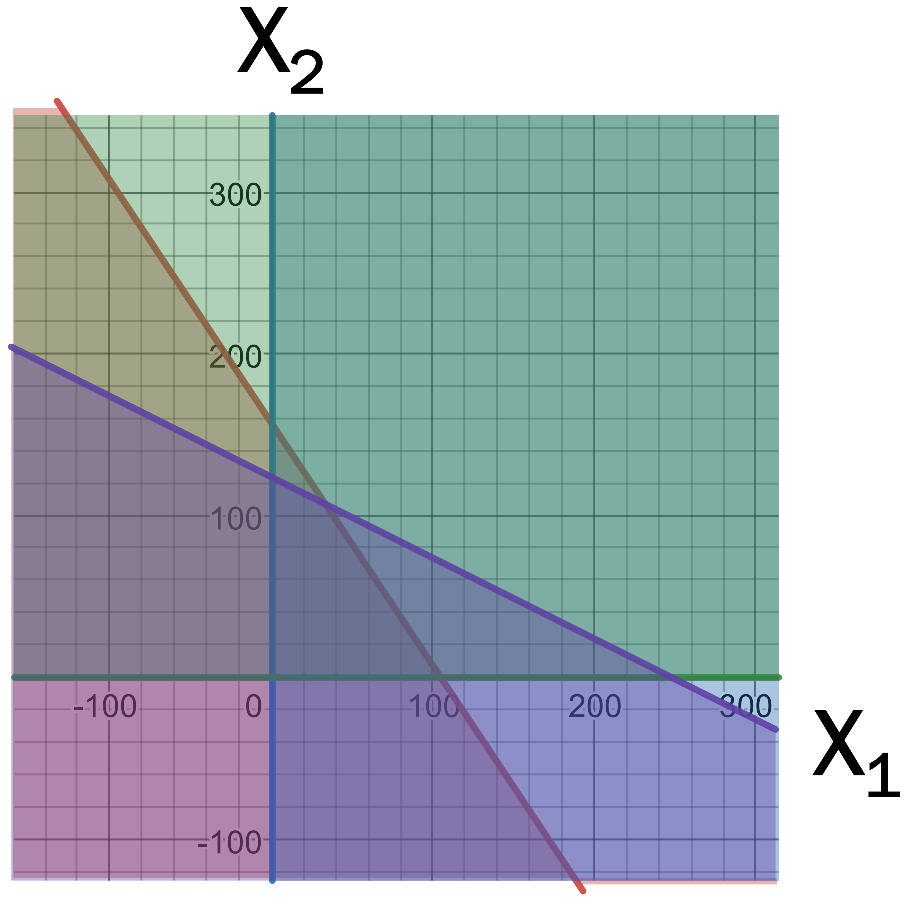
Feasible region

$X_1 \geq 0$

$X_2 \geq 0$

$15X_1 + 10X_2 \leq 1566$

$1X_1 + 2X_2 \leq 250$



Feasible region

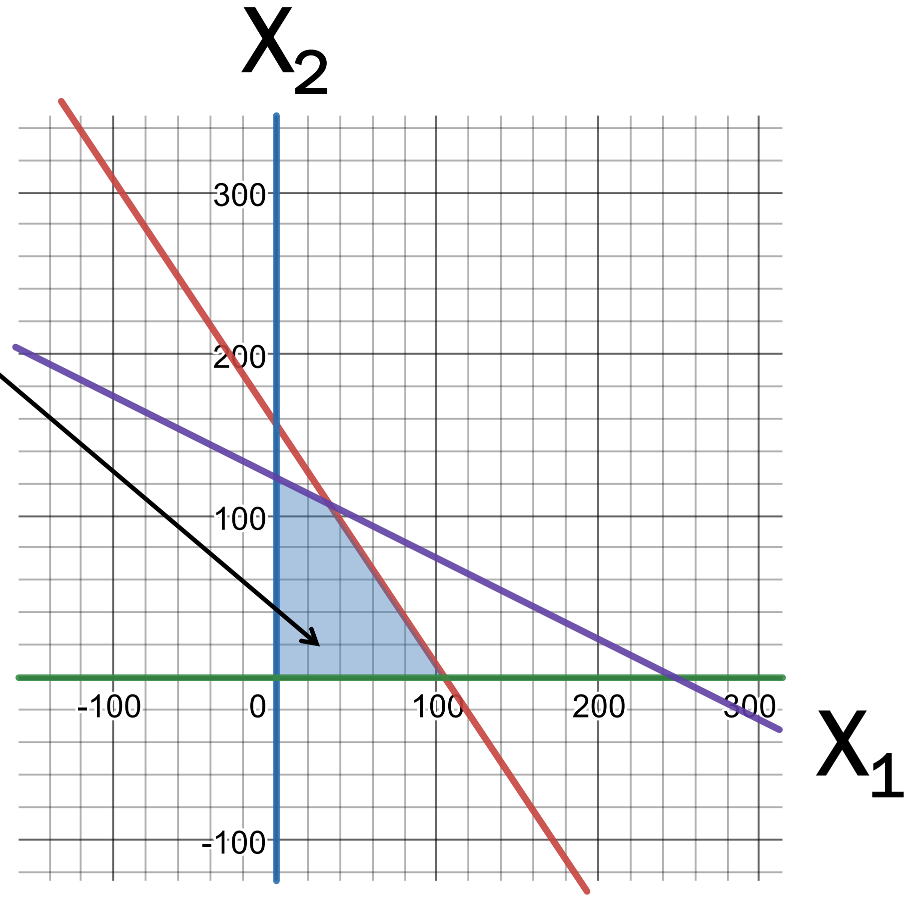
$X_1 \geq 0$

$X_2 \geq 0$

$15X_1+10X_2 \leq 1566$

$1X_1+2X_2 \leq 250$

Any (X_1, X_2) within these bounds is a feasible solution



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Feasible region

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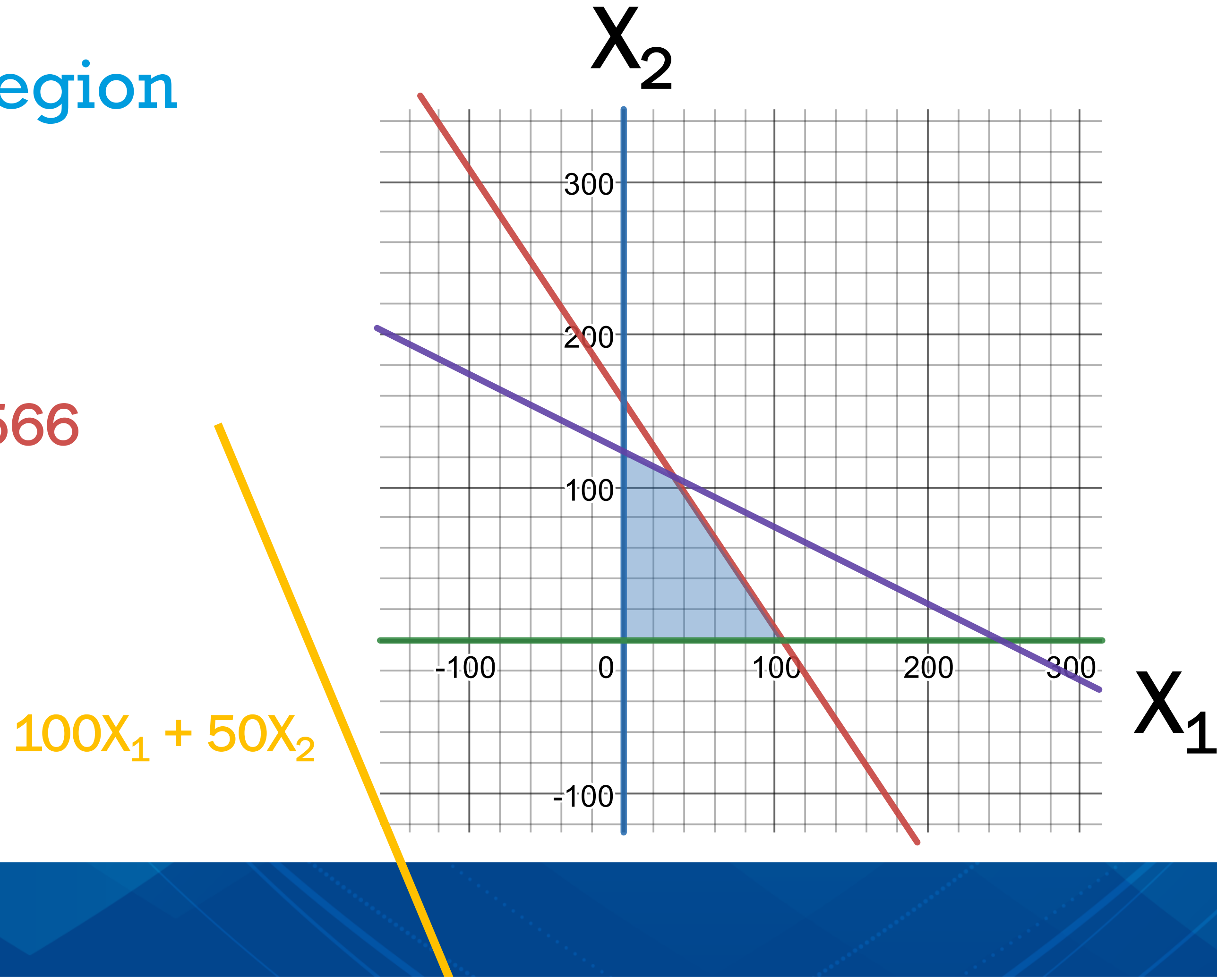

Feasible region

$X_1 \geq 0$

$X_2 \geq 0$

$15X_1 + 10X_2 \leq 1566$

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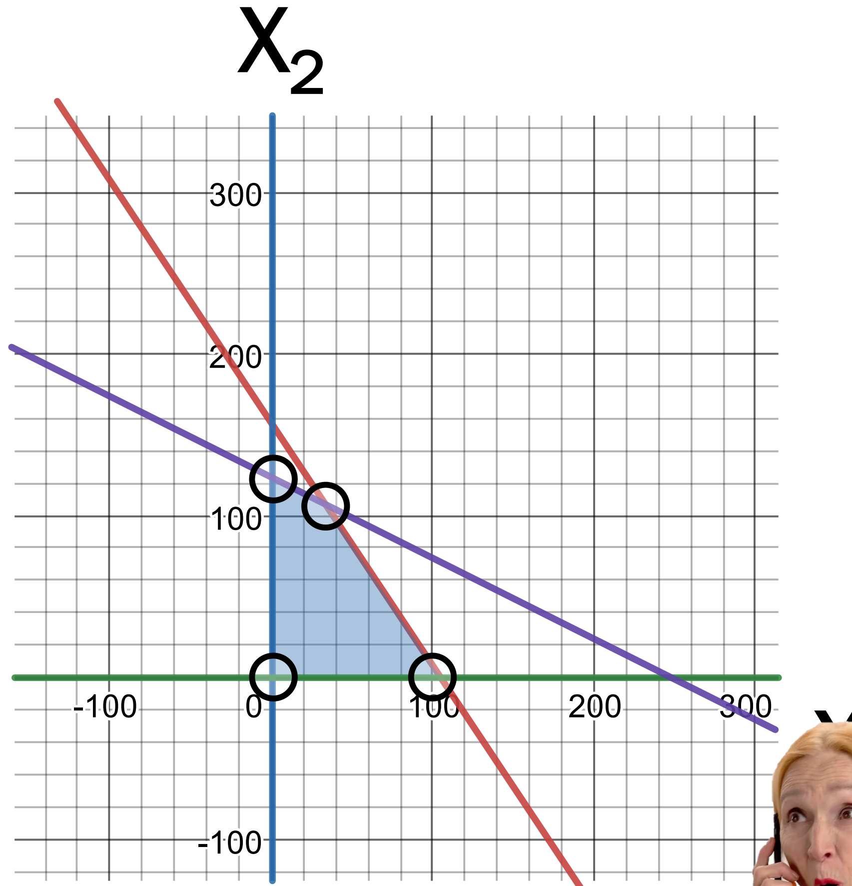
Optimal solution will be at one of the corner points, calculate using $100X_1 + 50X_2$



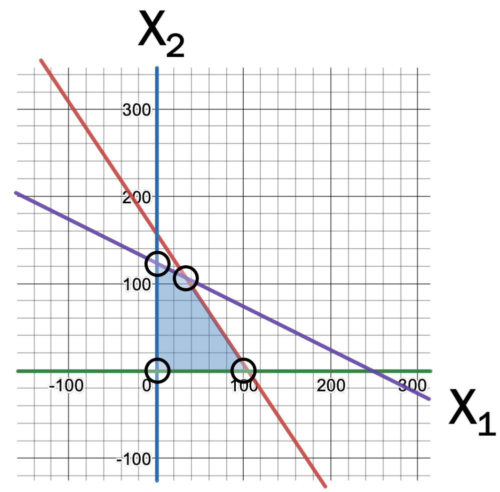
Depending on the type of problem, different optimization methods might (not) be appropriate

Linear programming	• All model functions are linear
Goal programming	• Model includes multiple objectives
Integer programming	• Decision variables must be integers
Non-linear programming	• Any of the model functions is non-linear

* This is a non-exhaustive list of mathematical programming approaches

Particular challenges introduced by non-linearity

1. **The optimal solution is NOT necessarily on the boundary of the feasible region.**
   To solve nonlinear programming models we need to consider all solutions in the feasible region.



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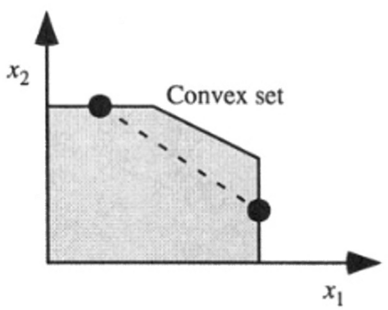
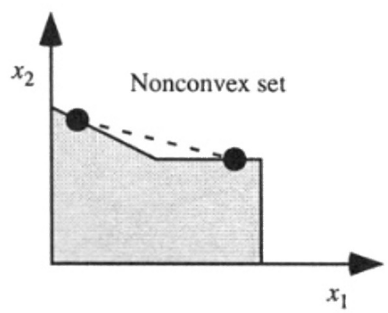
Sarker, R., Mohammadian, M., Yao, X. (Eds.), 2002. Evolutionary Optimization, International Series in Operations Research & Management Science. Springer US.

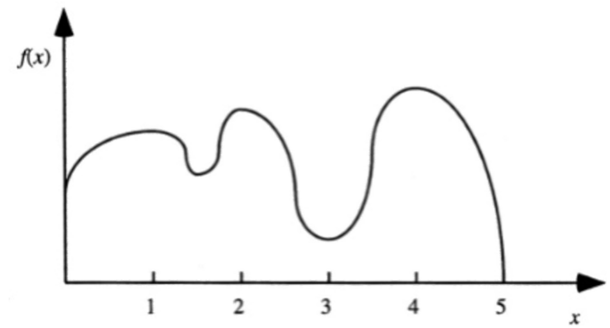
Particular challenges introduced by non-linearity

1. **The optimal solution is NOT necessarily on the boundary of the feasible region.**
   To solve nonlinear programming models we need to consider all solutions in the feasible region.

2. **A local maximum (or minimum) need not be a global maximum (or minimum). It is hard to guarantee that a local max is also a global max, because we cannot linearly interpolate between two points.**







Sarker, R., Mohammadian, M., Yao, X. (Eds.), 2002. Evolutionary Optimization, International Series in Operations Research & Management Science. Springer US.

Particular challenges introduced by non-linearity

1. **The optimal solution is NOT necessarily on the boundary of the**

f

T

s

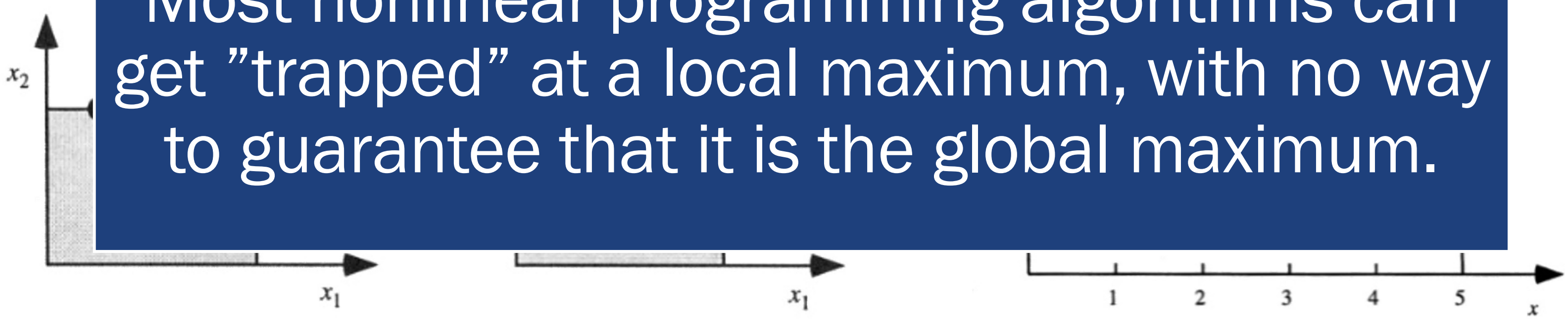
2. **A … or**

I … l

I

There is several different algorithms but no single algorithm can address all kinds of problems.

Most nonlinear programming algorithms can get ”trapped” at a local maximum, with no way to guarantee that it is the global maximum.



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Complex systems also face other complications

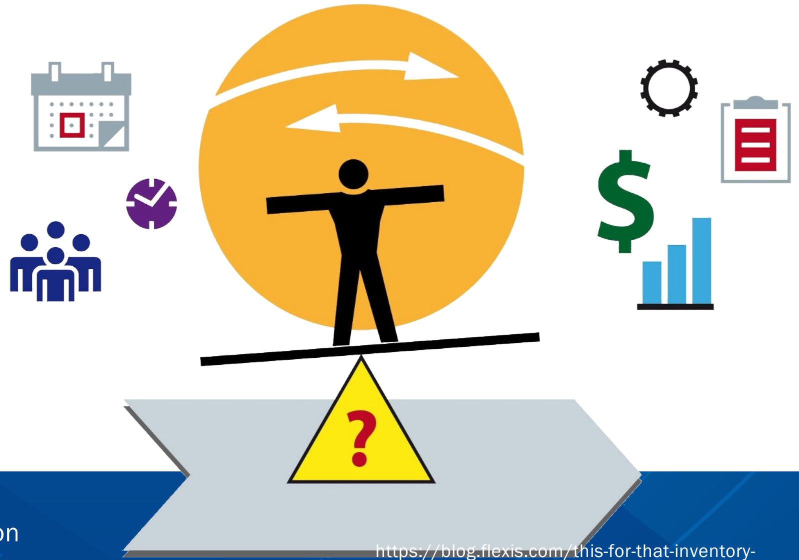
- **Uncertainty and stochasticity**
- **Many objectives for which we haven't perfectly articulated preferences**
- **Large number of decision variables and management options**

In complex systems, it is more common to use (multi-objective) optimization methods that use many simulations of how the system would perform with various alternative designs and operating procedures

Multi-objective optimization

Addresses optimization problems involving **more than one objective function to be optimized simultaneously.**

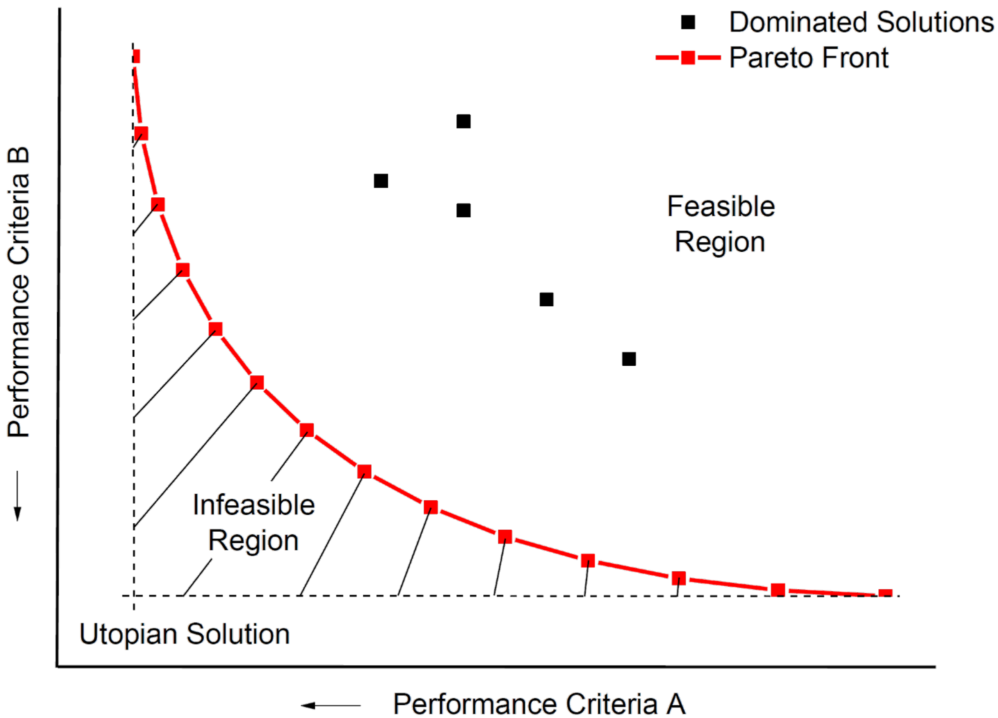
It has been applied in many fields of science, including engineering, economics and logistics where optimal decisions need to be taken in the **presence of trade-offs between two or more conflicting objectives.**



https://en.wikipedia.org/wiki/Multi-objective_optimization

https://blog.flexis.com/this-for-that-inventory-management-and-trade-offs-in-todays-supply-chain

Multi-objective optimization



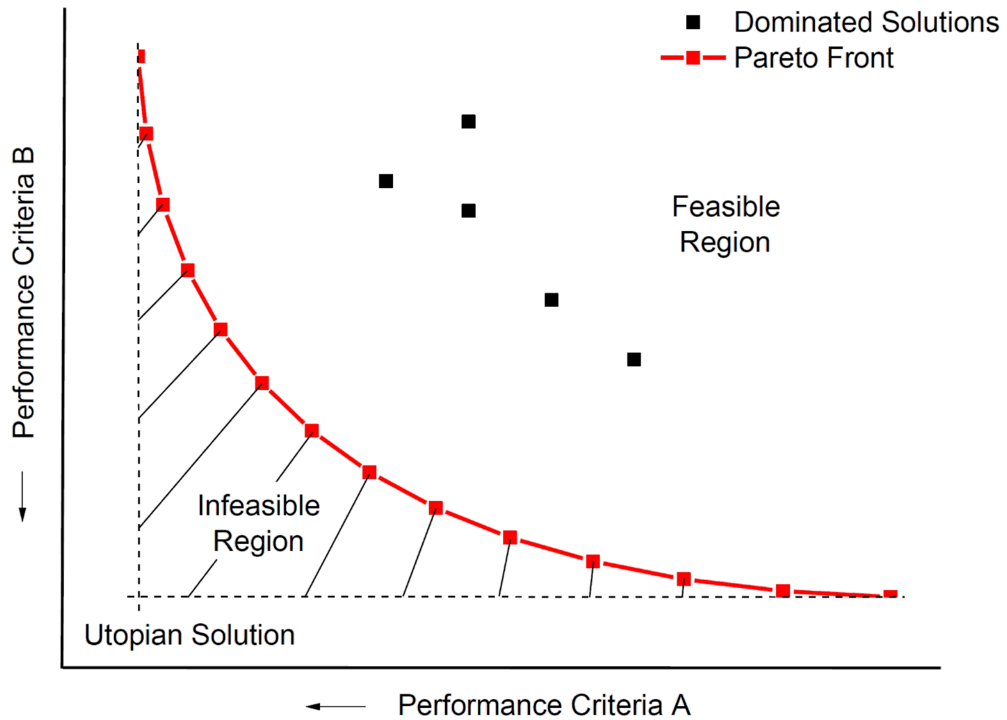
For most multi-objective optimization problems, **no single solution exists that simultaneously optimizes each objective**.

In that case, the objective functions are said to be **conflicting**.

https://www.mathworks.com/matlabcentral/fileexchange/66588-multi-objective-optimization-algorithm-for-expensive-to-evaluate-function

https://en.wikipedia.org/wiki/Multi-objective_optimization

Multi-objective optimization



<u>Used not just for finding ‘optimal’ solutions:</u>

- Understand range of representative/possible solutions
- Identify conflicts between objectives
- Quantify tradeoffs between objectives
- Navigate alternative decision-maker preferences on the objectives

Difference from Goal Programming*

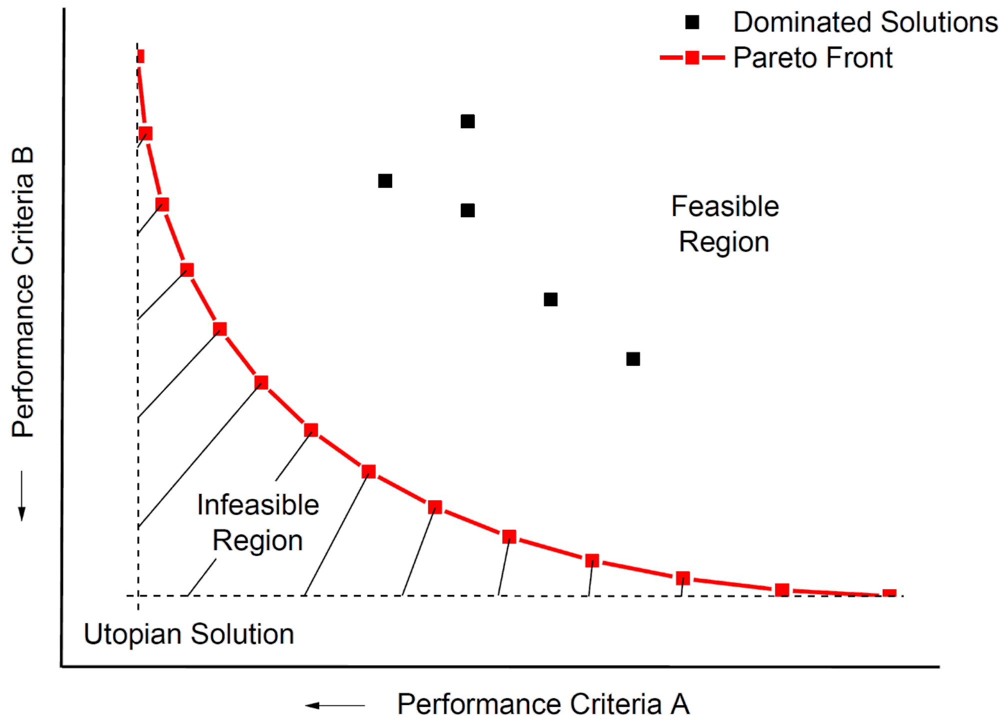
A priori	*A posteriori*
• *'from what is before'* • Objective preference is articulated **before** searching for solutions • Preferences are used to **weigh objectives** in a utility function	• *'from what comes after'* • Objective preference is articulated **after** searching for solution • Preferences can be used to **navigate the identified solutions**

* and similar *a priori* approaches

General criticisms of *a priori* approaches

- Strong assumption of expertise and familiarity with the problem to articulate preferences
- Hard to know what you prefer before you know what you can get
- Limit the solution space without knowledge of what all options look like
- Different stakeholders in a system might have different preferences

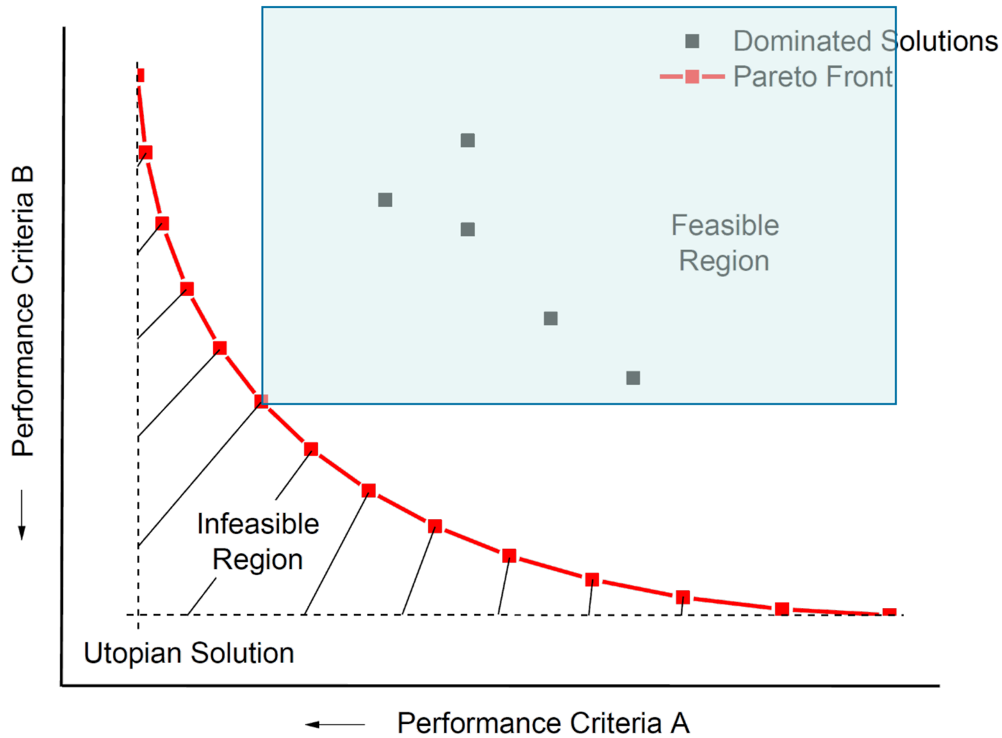
Multiobjective Evolutionary Algorithms



Use mechanisms inspired by biological evolution (reproduction, mutation, selection, etc.) to ***evolve*** a set of candidate solutions towards the Pareto front.

https://www.mathworks.com/matlabcentral/fileexchange/66588-multi-objective-optimization-algorithm-for-expensive-to-evaluate-function

Multiobjective Evolutionary Algorithms

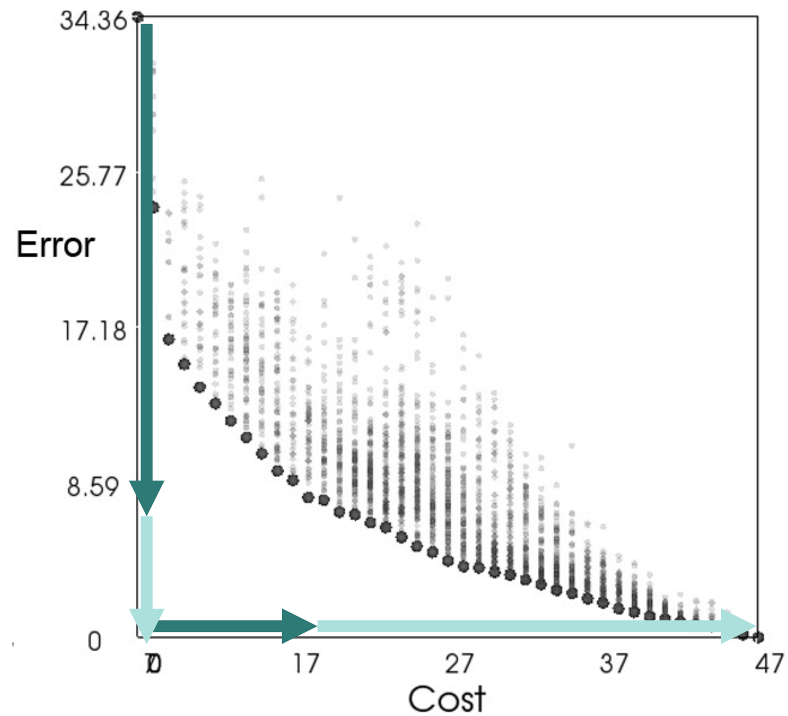


A solution is called nondominated (or Pareto optimal) if none of the objective functions can be improved in value without degrading some of the other objective values.

Multiobjective Evolutionary Algorithms

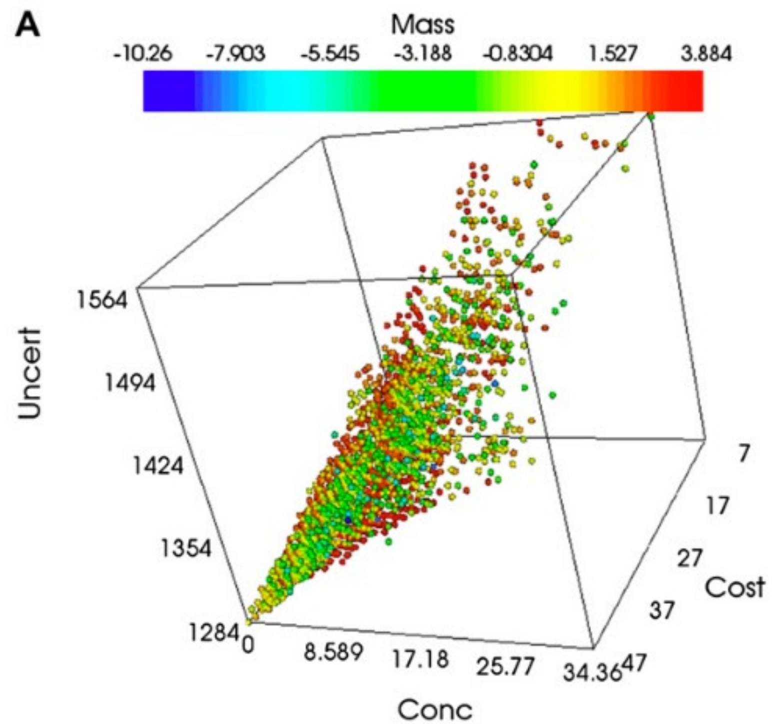
We can use the set of non-dominated solutions to assess tradeoffs and conflicts between our objectives:

- Small increases in **Cost** initially result in big **Error** decreases
- Further decreases in **Error** require big increases in **Cost**



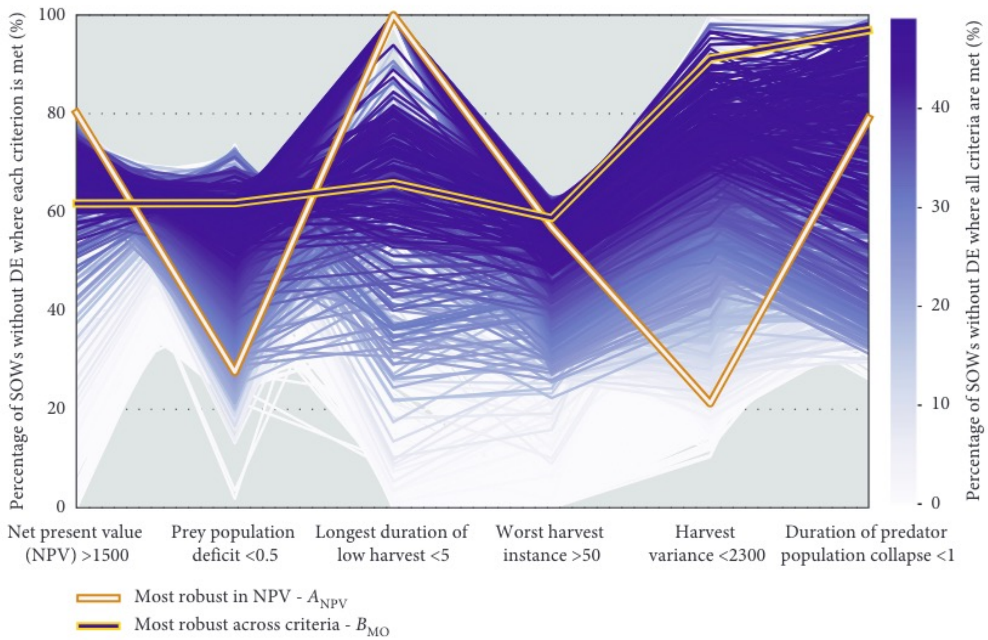
Multiobjective Evolutionary Algorithms

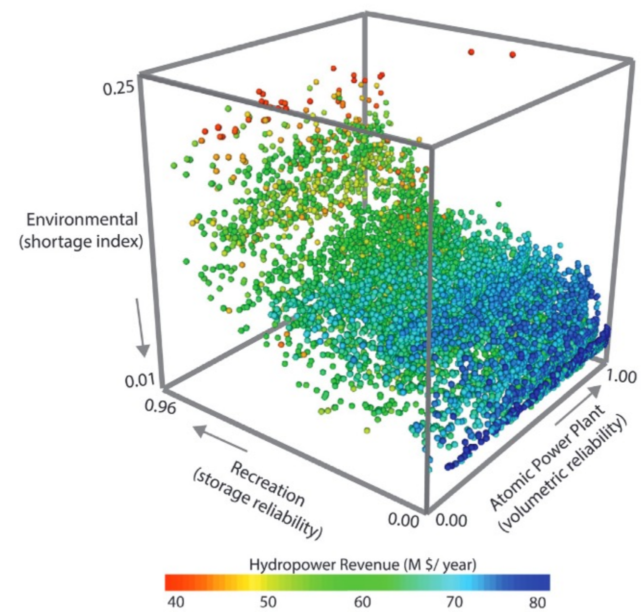
With the inclusion of additional objectives, we can make similar explorations across multiple goals we might have for the system.



Kollat, J.B., Reed, P., 2007
https://doi.org/10.1016/j.envsoft.2007.02.001

Visual analytics are central to such analyses





https://www.hindawi.com/journals/complexity/2020/4170453/

https://doi.org/10.1016/j.advwatres.2016.04.006

Topics for discussion

- How do we balance between modeling the right things and modeling things right?
- How do such choices affect the decisions we (can) make?
- What kinds of decision problems do you face in your work? What are the opportunities or limitations to use these methods?

Thank you! Here's some useful links:

- Open source Multiobjective Evolutionary Algorithms and other tools: http://moeaframework.org/
- Open source Python Package for MO optimization and other cool stuff (including visualization tools): https://github.com/Project-Platypus
- Useful blog with practical tutorials on multiobjective optimization: http://waterprogramming.wordpress.com/

- Personal website: https://www.hadjimichael.info/
- Email me to say hi: hadjimichael@psu.edu

Additional Useful Reading

- Hillier, F.S., and G.J. Lieberman (2001). Introduction to Operations Research, 7th ed., McGraw-Hill, Burr Ridge, IL.
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