Explainable Multicriteria Optimization
meets
Life-Science Applications

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Contact me … (m.t.m.emmerich@liacs.leidenuniv.nl) … if

- You have an interesting network simulation/optimization problem
- You have an interesting design problem with multiple criteria

- Goal:
  - Big scale: Write proposal for a tandem grant (2 PhD) on explainable (XAI) black box simulation and/or multicriteria optimization with application in the life sciences.
  - Small scale: Master thesis/Bachelor thesis proposals on a pilot in these directions; collaboration with supervision of PhD or Master Student.

1/2 Managing Complex Networks

What we can offer

- Efficient CTMC simulation of the contact process (infectious disease)
- Identification of parameters in complex networks (Bacillus subtilis, gene regulatory networks)
- Applying multicriteria optimization to problems of network identification and management
- **Explainable AI & Analytics (new)**
  ➔ proposal

What we are looking for

- Challenging problems with network data to be analyzed and some aspect of optimization or simulation
- E.g.:
  - Molecular data
  - Chemical reactions networks/metabolic networks
  - Epidemiological data

2/2 Explainable Multicriteria Optimization

What we can offer

- Groundbreaking new methods that explain the results of multicriteria search or design problems

- Explanations (per criterion)
  - What variables/features influence which criterion?
  - Which data is important to support a prediction?
  - Contingency management
  - Trade-off explanations

What we look for

- Search/Optimization problems in the life sciences

- Optimal design of
  - Plants
  - Molecules
  - Proteins
  - Mixtures
  - Geometrical Structures
  - Interventions
  - …