

# MooViE: Multi-objective optimization Visualization Engine

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## Multi-objective Experimental Design for $^{13}\text{C}$ Metabolic Flux Analysis

In  $^{13}\text{C}$  Metabolic Flux Analysis microorganisms are fed with a  $^{13}\text{C}$ -labeled substrate. The labeling incorporation within the cell is then used to infer the internal metabolic reaction rates, called fluxes. Different substrates are available that influence how well the fluxes can be determined. Finding an optimal substrate mixture is a multi-objective problem, because there are several ways to define the quality of a substrate and cost consideration play also a role. Since these objectives are conflicting, no single optimal solution but a set of compromises exists, in which it is not possible to improve one objective without changing other objectives to the worse. These design are called Pareto optimal.

### Evaluating Multi-objective Experimental Design Data

The high dimensionality and density of the design solutions raise the need for a suitable visualization technique that allows in-depth inspection of the data. That is:

- accessing conflicts in the objectives
- connecting the mixture design to the objectives
- supporting the selection process

Since the available approaches (e.g. scatter plots, parallel coordinates, dimension reduction) fail here, a new approach is created.

## A novel visualization scheme: MooViE

MooViE, our new approach for visualization of high-volume multi-objective data is:

### Intuitive

Two dimensional graphics that uses established visualization elements

### Information rich

Visualization of relationship between the objectives, mapping of substrates to objectives and substrate frequency

### Visually appealing

Aesthetically pleasing circular layout with carefully selected colors

### Versatile

Dedicated techniques for sparse datasets and the case of two objectives

### Fast

Lightweight C++11 codebase utilizing the cairo (cairographics.org) library

## Beyond Metabolic Flux Analysis

MooViE can handle data from any multi-objective optimization, or arbitrary high dimensional mapping. We have used MooViE to visualize:

- a large-scale MO-ED study, comparing the performance of different analytic platforms
- results of a multi-objective parameter estimation for chromatography simulation
- a parameter study for a Monte Carlo based single cell tracker

### Interactive features

MooViE will be extended by interactive features:

- selecting and highlighting specific solutions
- choosing data subsets by context dependent prefiltering
- reordering and rescaling the objectives

### Image statistics

- 10 substrates
- 4 objectives
- 3 quality measures (D-, A-, E-criterion)
- costs
- 1000+ Pareto solutions
- 90 megapixel resolution
- Image creation with circos (circos.ca)

### 2 Relationship between the objectives

The values of the first objective are color coded and this color is transferred to the other objectives. This allows an easy comparison of the secondary objectives to the first one.

### 3 Substrates and their frequency

Each substrate axis is drawn as a circular segment. Histograms on top of the segments depict how often the specific substrate fraction is used in the Pareto designs.

### 4 Mapping substrates to objectives

Every single mapping is represented by an ensemble of arches. For every utilized substrate an arch connects the fractional value of the substrate to the first objective value.

### 1 Tracing the values of the objectives

The objective axes are represented by a set of concentric semicircles. Lines connect neighboring objectives and elucidate their relationship, while boxes highlight the objective values.



**Software**

<https://github.com/modsim/MooViE>

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