Tyche Release 0.1.0

National Renewable Energy Laboratory

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Risk and uncertainty are core characteristics of research and development (R&D) programs. Attempting to do what has not been done before will sometimes end in failure, just as it will sometimes lead to extraordinary success. The challenge is to identify an optimal mix of R&D investments in pathways that provide the highest returns while reducing the costs of failure. The goal of the R&D Pathway and Portfolio Analysis and Evaluation project is to develop systematic, scalable pathway and portfolio analysis and evaluation methodologies and tools that provide high value to the U.S. Department of Energy (DOE) and its Office of Energy Efficiency & Renewable Energy (EERE). This work aims to assist analysts and decision makers identify and evaluate, quantify and monitor, manage, document, and communicate energy technology R&D pathway and portfolio risks and benefits. The project-level risks typically considered are technology cost and performance (e.g., efficiency and environmental impact), while the portfolio level risks generally include market factors (e.g., competitiveness and consumer preference).

This documentation summarizes work in progress on R&D Portfolio Analysis and Evaluation. It discusses a mock FOA approach for designing a decision-support process for R&D portfolios, the portfolio-optimization methodology, and the underlying software framework. The end goal of this process is to inform decision-making across R&D projects and programs through identifying and evaluating, quantifying, and monitoring, managing, documenting, and communicating energy technology R&D pathway and portfolio risks and benefits.

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CHAPTER

ONE

APPROACH

Our production-function approach to R&D portfolio evaluation is mathematically formulated as a stochastic multiobjective decision-optimization problem and is implemented in the Python programming language. The framework abstracts the technology-independent aspects of the problem into a generic computational schema and enables the modeler to specify the technology-dependent aspects in a set of data tables and Python functions. This approach not only minimizes the labor needed to add new technologies, but it also enforces uniformity of financial, mass-balance, and other assumptions in the analysis.

The framework is scalable, supporting rapid computation on laptops computer and large-ensemble studies on high-performance computers (HPC). The use of vectorized operations for the stochastic calculations and of response-surface fits for the portfolio evaluations minimizes the computational resources needed for complex multi-objective optimizations. The software handles parameterized studies such as tornado plots, Monte-Carlo sensitivity analyses, and a generalization of epsilon-constraint optimization.

All values in the data tables may be probability distributions, specified by Python expressions using a large library of standard distributions, or the values may be simple numbers. Expert opinion is encoded through these distributions. The opinions may be combined prior to simulator or subsequent to it.

Four example technologies have been implemented as examples illustrating framework's use: biorefineries, electrolysis, residential photovoltaics (PV), and utility-scale PV. A desktop user interface allows exploration of the cost-benefit trade-offs in portfolio decision problems.

Below we detail the mathematical formulation and its implementation as a Python module with user-specified data tables and technology functions. We also provide a sample analysis that exercises the framework's main features.

MATHEMATICAL FORMULATION

We separate the financial and conversion-efficiency aspects of a production process, which are generic across all technologies, from the physical and technical aspects, which are necessarily specific to the particular process. The motivation for this is that the financial and waste computations can be done uniformly for any technology (even for disparate ones such as PV cells and biofuels) and that different experts may be required to assess the cost, waste, and techno-physical aspects of technological progress. Table 2.1 defines the indices that are used for the variables that are defined in Table 2.2.

Table 2.1: Definitions for set indices used for variable subscripts.

Set	Description	Examples
$c \in \mathcal{C}$	capital	equipment
$f \in \mathcal{F}$	fixed cost	rent, insurance
$i \in \mathcal{I}$	input	feedstock, labor
$o \in \mathcal{O}$	output	product, co-product, waste
$m \in \mathcal{M}$	metric	cost, jobs, carbon footprint, efficiency, lifetime
$p \in \mathcal{P}$	technical parameter	temperature, pressure
$\nu \in N$	technology type	electrolysis, PV cell
$\theta \in \Theta$	scenario	the result of a particular investment
$\chi \in X$	investment category	investment alternatives
$\phi \in \Phi_{\chi}$	investment	a particular investment
$\omega \in \Omega$	portfolio	a basket of investments

Table 2.2: Definitions for variables.

Variable	Туре	Description	Units
K	calculated	unit cost	USD/unit
C_c	function	capital cost	USD
$ au_c$	cost	lifetime of capital	year
S	cost	scale of operation	unit/year
F_f	function	fixed cost	USD/year
I_i	input	input quantity	input/unit
I_i^*	calculated	ideal input quantity	input/unit
η_i	waste	input efficiency	input/input
p_i	cost	input price	USD/input
O_o	calculated	output quantity	output/unit
O_o^*	calculated	ideal output quantity	output/unit
η_o'	waste	output efficiency	output/output
p'_o	cost	output price (+/-)	USD/output
μ_m	calculated	metric	metric/unit
P_o	function	production function	output/unit

Continued on next page

Variable	Туре	Description	Units
M_m	function	metric function	metric/unit
α_p	parameter	technical parameter	(mixed)
ξ_{θ}	variable	scenario inputs	(mixed)
ζ_{θ}	variable	scenario outputs	(mixed)
ψ	function	scenario evaluation	(mixed)
σ_{ϕ}	function	scenario probability	1
q_{ϕ}	variable	investment cost	USD
ζ_{ϕ}	random variable	investment outcome	(mixed)
$\mathbf{Z}(\omega)$	random variable	portfolio outcome	(mixed)
$Q(\omega)$	calculated	portfolio cost	USD
Q^{\min}	parameter	minimum portfolio cost	USD
Qmax	parameter	maximum portfolio cost	USD
$q_{\phi}^{ ext{min}}$	parameter	minimum category cost	USD
q_{ϕ}^{max}	parameter	maximum category cost	USD
Z^{\min}	parameter	minimum output/metric	(mixed)
Z^{\max}	parameter	maximum output/metric	(mixed)
F, G	operator	evaluate probabilities	(mixed)

Table 2.2 - continued from previous page

2.1 Cost

The cost characterizations (capital and fixed costs) are represented as functions of the scale of operations and of the technical parameters in the design:

• Capital cost: $C_c(S, \alpha_p)$.

• Fixed cost: $F_f(S, \alpha_p)$.

The per-unit cost is computed using a simple levelization formula:

$$K = \left(\sum_{c} C_{c} / \tau_{c} + \sum_{f} F_{f}\right) / S + \sum_{i} p_{i} \cdot I_{i} - \sum_{o} p'_{o} \cdot O_{o}$$

2.2 Waste

The waste relative to the idealized production process is captured by the η parameters. Expert elicitation might estimate how the η s would change in response to R&D investment.

• Waste of input: $I_i^* = \eta_i I_i$.

• Waste of output: $O_o = \eta'_o O_o^*$.

2.3 Production

The production function idealizes production by ignoring waste, but accounting for physical and technical processes (e.g., stoichiometry). This requires a technical model or a tabulation/fit of the results of technical modeling.

$$O_o^* = P_o(S, C_c, \tau_c, F_f, I_i^*, \alpha_p)$$

2.4 Metrics

Metrics such as efficiency, lifetime, or carbon footprint are also compute based on the physical and technical characteristics of the process. This requires a technical model or a tabulation/fit of the results of technical modeling. We use the convention that higher values are worse and lower values are better.

$$\mu_m = M_m(S, C_c, \tau_c, F_f, I_i, I_i^*, O_o^*, O_o, K, \alpha_p)$$

2.5 Scenarios

A scenario represents a state of affairs for a technology ν . If we denote the scenario as θ , we have the tuple of input variables

$$\xi_{\theta} = (S, C_c, \tau_c, F_f, I_i, \eta_i, \eta_o', \alpha_p, p_i, p_o')|_{\theta}$$

and the tuple of output variables

$$\zeta_{\theta} = (K, I_i^*, O_o^*, O_o, \mu_m)|_{\theta}$$

and their relationship

$$\zeta_{\theta} = \psi_{\nu} \left(\xi_{\theta} \right) |_{\nu = \nu(\theta)}$$

given the tuple of functions

$$\psi_{\nu} = (P_o, M_m)|_{\nu}$$

for the technology of the scenario.

2.6 Investments

An *investment* ϕ assigns a probability distribution to scenarios:

$$\sigma_{\phi}(\theta) = P(\theta|\phi).$$

such that

$$\int d\theta \sigma_{\phi}(\theta) = 1 \text{ or } \sum_{\theta} \sigma_{\phi}(\theta) = 1,$$

depending upon whether one is performing the computations discretely or continuously. Expectations and other measures on probability distributions can be computed from the $\sigma_{\phi}(\theta)$. We treat the outcome ζ_{ϕ} as a random variable for the outcomes ζ_{θ} according to the distribution $\sigma_{\phi}(\theta)$.

Because investment options may be mutually exclusive, as is the case for investing in the same R&D at different funding levels, we say Φ_{χ} is the set of mutually exclusive investments (i.e., only one can occur simultaneously) in investment category χ : investments in different categories χ can be combined arbitrarily, but just one investment from each Φ_{χ} may be chosen.

2.3. Production 7

Thus the universe of all portfolios is $\Omega = \prod_{\chi} \Phi_{\chi}$, so a particular portfolio $\omega \in \Omega$ has components $\phi = \omega_{\chi} \in \Phi_{\chi}$. The overall outcome of a portfolio is a random variable:

$$\mathbf{Z}(\omega) = \sum_{\chi} \zeta_{\phi} \mid_{\phi = \omega_{\chi}}$$

The cost of an investment in one of the constituents ϕ is q_{ϕ} , so the cost of a portfolio is:

$$Q(\omega) = \sum_{\chi} q_{\phi} \mid_{\phi = \omega_{\chi}}$$

2.7 Decision problem

The multi-objective decision problem is

$$\min_{\omega \in \Omega} \mathbb{F} \mathbf{Z}(\omega)$$

such that

$$Q^{\min} \leq Q(\omega) \leq Q^{\max}$$
,

$$q_\phi^{\rm min} \leq q_{\phi=\omega_\chi} \leq q_\phi^{\rm max}$$
 ,

$$Z^{\min} \leq \mathbb{G} \mathbf{Z}(\omega) \leq Z^{\max}$$
,

where \mathbb{F} and \mathbb{G} are the expectation operator \mathbb{E} , the value-at-risk, or another operator on probability spaces. Recall that \mathbf{Z} is a vector with components for cost K and each metric μ_m , so this is a multi-objective problem.

The two-stage decision problem is a special case of the general problem outlined here: Each scenario θ can be considers as a composite of one or more stages.

2.8 Experts

Each expert elicitation takes the form of an assessment of the probability and range (e.g., 10th to 90th percentile) of change in the cost or waste parameters or the production or metric functions. In essence, the expert elicitation defines $\sigma_{\phi}(\theta)$ for each potential scenario θ of each investment ϕ .

CHAPTER

THREE

ELECTROLYSIS EXAMPLE

Here is a very simple model for electrolysis of water. We just have water, electricity, a catalyst, and some lab space. We choose the fundamental unit of operation to be moles of H_2 :

$$H_2O \to H_2 + \frac{1}{2}O_2$$

Experts could assess how much R&D to increase the various efficiencies η would cost. They could also suggest different catalysts, adding alkali, or replacing the process with PEM.

3.1 Tracked quantities.

```
\mathcal{C} = \{catalyst\}
\mathcal{F} = \{rent\}
\mathcal{I} = \{water, electricity\}
\mathcal{O} = \{oxygen, hydrogen\}
\mathcal{M} = \{jobs\}
```

3.2 Current design.

```
\begin{split} I_{\text{water}} &= 19.04 \text{ g/mole} \\ \eta_{\text{water}} &= 0.95 \text{ (due to mass transport loss on input)} \\ I_{\text{electricity}} &= 279 \text{ kJ/mole} \\ \eta_{\text{electricity}} &= 0.85 \text{ (due to ohmic losses on input)} \\ \eta_{\text{oxygen}} &= 0.90 \text{ (due to mass transport loss on output)} \\ \eta_{\text{hydrogen}} &= 0.90 \text{ (due to mass transport loss on output)} \end{split}
```

3.3 Current costs.

$$C_{\mathrm{catalyst}} = (0.63~\mathrm{USD}) \cdot \frac{S}{6650~\mathrm{mole/yr}}$$
 (cost of Al-Ni catalyst)

 $\tau_{\text{catalyst}} = 3 \text{ yr (effective lifetime of Al-Ni catalyst)}$

$$F_{\text{rent}} = (1000 \text{ USD/yr}) \cdot \frac{S}{6650 \text{ mole/yr}}$$

S = 6650 mole/yr (rough estimate for a 50W setup)

3.4 Current prices.

$$p_{\mathrm{water}} = 4.8 \cdot 10^{-3} \; \mathrm{USD/mole}$$

$$p_{\text{electricity}} = 3.33 \cdot 10^{-5} \text{ USD/kJ}$$

$$p_{\rm oxygen} = 3.0 \cdot 10^{-3}~{\rm USD/g}$$

$$p_{\mathrm{hydrogen}} = 1.0 \cdot 10^{-2} \ \mathrm{USD/g}$$

3.5 Production function (à la Leontief)

$$P_{\rm oxygen} = (16.00~{\rm g}) \cdot \min \left\{ \tfrac{I_{\rm water}^*}{18.08~{\rm g}}, \tfrac{I_{\rm electricity}^*}{237~{\rm kJ}} \right\}$$

$$P_{ ext{hydrogen}} = (2.00 \text{ g}) \cdot \min \left\{ rac{I_{ ext{water}}^*}{18.08 \text{ g}}, rac{I_{ ext{electricity}}^*}{237 \text{ kJ}}
ight\}$$

3.6 Metric function.

$$M_{\rm cost} = K/O_{\rm hydrogen}$$

$$M_{\rm GHG} = \left(\left(0.00108~{\rm gCO2e/gH20} \right) I_{\rm water} + \left(0.138~{\rm gCO2e/kJ} \right) I_{\rm electricity} \right) / O_{\rm hydrogen}$$

$$M_{\rm jobs} = \left(0.00015~{\rm job/mole}\right)/O_{\rm hydrogen}$$

3.7 Performance of current design.

K = 0.18 USD/mole (i.e., not profitable since it is positive)

$$O_{\rm oxygen} = 14 \, {\rm g/mole}$$

$$O_{\text{hydrogen}} = 1.8 \text{ g/mole}$$

$$\mu_{\rm cost} = 0.102~{\rm USD/gH2}$$

$$\mu_{\mathrm{GHG}} = 21.4~\mathrm{gCO2e/gH2}$$

$$\mu_{\mathrm{jobs}} = 0.000083 \; \mathrm{job/gH2}$$

DATABASE SCHEMA

Database tables (one per set) hold all of the variables and the expert assessments. These tables are augmented by concise code with mathematical representations of the production and metric functions.

The Monte-Carlo computations are amenable to fast tensor-based implementation in Python.

See https://github.com/NREL/portfolio/tree/master/production-function/framework/code/tyche/ for the tyche package that computes cost, production, and metrics from a technology design.

Each analysis case is represented by a Technology and a Scenario within that technology. In the specifications for the individual tables, we use the simple electrolysis example to populate the table.

4.1 Metadata about indices

The indices table (see Table 4.1) simply describes the various indices available for the variables. The Offset column specifies the memory location in the argument for the production and metric functions.

Technology	Type	Index	Offset	Description	Notes
Simple electrolysis	Capital	Catalyst	0	Catalyst	
Simple electrolysis	Fixed	Rent	0	Rent	
Simple electrolysis	Input	Water	0	Water	
Simple electrolysis	Input	Electricity	1	Electricity	
Simple electrolysis	Output	Oxygen	0	Oxygen	
Simple electrolysis	Output	Hydrogen	1	Hydrogen	
Simple electrolysis	Metric	Cost	0	Cost	
Simple electrolysis	Metric	Jobs	1	Jobs	
Simple electrolysis	Metric	GHG	2	GHGs	

Table 4.1: Example of the indices table.

4.2 Design variables

The design table (see Table 4.2) specifies the values of all of the variables in the mathematical formulation of the design. Note that the Value column can either contain numeric literals or Python expressions specifying probability distribution functions. For example, a normal distribution with mean of five and standard deviation of two would be written st. norm(5, 2). All of the Scipy probability distribution functions are available for use, as are two special functions, constant and mixture. The constant distribution is just a single constant value; the mixture distribution is the mixture of a list of distributions, with specified relative weights. The mixture function is particularly important because it allows one to specify a first distribution in the case of an R&D breakthrough, but a second distribution if no breakthrough occurs.

		_			
Scenario	Variable	Index	Value	Units	Notes
Base	Input	Water	19.04	g/mole	$I_{ m water}$
Base	Input Efficiency	Water	0.95	1	$\eta_{ m water}$
Base	Input	Electricity	279	kJ/mole	$I_{ m electricity}$
Base	Input Efficiency	Electricity	0.85	1	$\eta_{ m electricity}$
Base	Output Efficiency	Oxygen	0.90	1	$\eta_{ m oxygen}$
Base	Output Efficiency	Hydrogen	0.90	1	$\eta_{ ext{hydrogen}}$
Base	Lifetime	Catalyst	3	yr	$ au_{ m catalyst}$
Base	Scale		6650	mole/yr	S
Base	Input price	Water	4.8e-3	USD/mole	p_{water}
Base	Input price	Electricity	3.33e-5	USD/kJ	$p_{ m electricity}$
Base	Output price	Oxygen	3.0e-3	USD/g	p_{oxygen}
Base	Output price	Hydrogen	1.0e-2	USD/g	$p_{hydrogen}$
	Base Base Base Base Base Base Base Base	Base Input Base Input Efficiency Base Input Base Input Efficiency Base Output Efficiency Base Output Efficiency Base Input Efficiency Base Output Efficiency Base Output Price Base Output price	Base Input Water Base Input Efficiency Water Base Input Electricity Base Input Efficiency Electricity Base Output Efficiency Oxygen Base Output Efficiency Hydrogen Base Lifetime Catalyst Base Scale Base Input price Water Base Input price Electricity Base Output price Oxygen	BaseInputWater19.04BaseInput EfficiencyWater0.95BaseInputElectricity279BaseInput EfficiencyElectricity0.85BaseOutput EfficiencyOxygen0.90BaseOutput EfficiencyHydrogen0.90BaseLifetimeCatalyst3BaseScale6650BaseInput priceWater4.8e-3BaseInput priceElectricity3.33e-5BaseOutput priceOxygen3.0e-3	BaseInputWater19.04g/moleBaseInput EfficiencyWater0.951BaseInputElectricity279kJ/moleBaseInput EfficiencyElectricity0.851BaseOutput EfficiencyOxygen0.901BaseOutput EfficiencyHydrogen0.901BaseLifetimeCatalyst3yrBaseScale6650mole/yrBaseInput priceWater4.8e-3USD/moleBaseInput priceElectricity3.33e-5USD/kJBaseOutput priceOxygen3.0e-3USD/g

Table 4.2: Example of the designs table.

4.3 Metadata for functions

The functions table (see Table 4.3) simply documents which Python module and functions to use for the technology and scenario. Currently only the numpy style of function is supported, but later plain Python functions and tensor-flow functions will be allowed.

Table 4.3: Example of the functions table.

Technology	Style	Module	Capital	Fixed	Production	Metrics	Notes
Simple electrolysis	numpy	simple_electrolysis	capital_cost	fixed_cost	production	metrics	

4.4 Parameters for functions

The parameters table (see Table 4.4) contains ad-hoc parameters specific to the particular production and metrics functions. The Offset column specifies the memory location in the argument for the production and metric functions.

Technology Sce-Parameter Off-Value Units Notes nario set Simple Base Oxygen production 0 16.00 elecg trolysis Simple 2.00 elec-Base Hydrogen production 1 g trolysis Simple elec-Base Water consumption 2 18.08 g trolysis Simple elec-Base Electricity consumption 3 237 kJ trolysis Simple Base Jobs 4 1.5ejob/mole electrolysis Base 6650 Simple elec-Reference scale 5 mole/yr trolysis USD Simple Reference capital cost for 0.63 elec-Base 6 trolysis catalyst Simple elec-Base Reference fixed cost for 7 1000 USD/yr trolysis rent based on 244,956 gallons = 1 GHG factor for water 8 Simple elec-Base 0.00108 gCO2e/g trolysis Mg CO2e Simple elec-Base GHG factor for electricity 9 0.138 gCO2e/k based on 1 kWh = 0.5 kg CO2e trolysis

Table 4.4: Example of the parameters table.

4.5 Units for results

The results table (see Table 4.5) simply specifies the units for the results.

Variable Units Technology Index Notes Simple electrolysis Cost Cost USD/mole Simple electrolysis Output Oxygen g/mole Simple electrolysis Output Hydrogen g/mole Simple electrolysis Metric Cost job/gH2 Simple electrolysis Metric Jobs job/gH2 Simple electrolysis Metric GHG gCO2e/gH2

Table 4.5: Example of the results table.

4.6 Tranches of investments.

In the tranches table (see Table 4.6), each *category* of investment contains a set of mutually exclusive *tranches* that may be associated with one or more *scenarios* defined in the designs table. Typically, a category is associated with a technology area and each tranche corresponds to an investment strategy within that category.

4.5. Units for results

Table 4.6: Example of the tranches table.

Category	Tranche	Scenario	Amount	Notes
Electrolysis R&D	No Electrolysis R&D	Base Electrolysis	0	
Electrolysis R&D	Low Electrolysis R&D	Slow Progress on Electrolysis	1000000	
Electrolysis R&D	Medium Electrolysis R&D	Moderate Progress on Electrolysis	2500000	
Electrolysis R&D	High Electrolysis R&D	Fast Progress on Electrolysis	5000000	

4.7 Investments

In the investments table (see Table 4.7), each *investment* is associated with a single *tranche* in one or more *categories*. An investment typically combines tranches from several different investment categories.

Table 4.7: Example of the investments table.

Investment	Category	Tranche	Notes
No R&D Spending	Electrolysis R&D	No Electrolysis R&D	
Low R&D Spending	Electrolysis R&D	Low Electrolysis R&D	
Medium R&D Spending	Electrolysis R&D	Medium Electrolysis R&D	
High R&D Spending	Electrolysis R&D	High Electrolysis R&D	

DEFINING TECHNOLOGIES

Each technology design requires a Python module with a capital cost, a fixed cost, a production, and a metrics function. Listing 5.1 shows these functions for the simple electrolysis example.

Listing 5.1: Example technology-defining functions.

```
# Simple electrolysis.
# All of the computations must be vectorized, so use `numpy`.
import numpy as np
# Capital-cost function.
def capital_cost(
  scale,
  parameter
):
  # Scale the reference values.
  return np.stack([np.multiply(
    parameter[6], np.divide(scale, parameter[5])
  )])
# Fixed-cost function.
def fixed_cost(
  scale,
  parameter
  # Scale the reference values.
  return np.stack([np.multiply(
   parameter[7],
   np.divide(scale, parameter[5])
  )])
# Production function.
def production(
  capital,
  fixed,
  input,
  parameter
):
```

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```
# Moles of input.
 water = np.divide(input[0], parameter[2])
 electricity = np.divide(input[1], parameter[3])
  # Moles of output.
 output = np.minimum(water, electricity)
  # Grams of output.
 oxygen = np.multiply(output, parameter[0])
 hydrogen = np.multiply(output, parameter[1])
 # Package results.
 return np.stack([oxygen, hydrogen])
# Metrics function.
def metrics(
 capital,
 fixed,
 input_raw,
 input,
 img/output_raw,
 output,
 cost,
 parameter
  # Hydrogen output.
 hydrogen = output[1]
 # Cost of hydrogen.
 cost1 = np.divide(cost, hydrogen)
 # Jobs normalized to hydrogen.
 jobs = np.divide(parameter[4], hydrogen)
 # GHGs associated with water and electricity.
 water = np.multiply(input_raw[0], parameter[8])
 electricity = np.multiply(input_raw[1], parameter[9])
 co2e = np.divide(np.add(water, electricity), hydrogen)
 # Package results.
 return np.stack([cost1, jobs, co2e])
```

OPTIMIZATION

6.1 Summary

Technology models and data are defined before the optimizer is called. Three methods in the <code>EpsilonConstraintOptimizer</code> class, <code>maximize_slsqp</code>, <code>maximize_shgo</code> and <code>maximize_diffev</code>, are wrappers for the algorithm calls. The optimization methods define the optimization problem according to each algorithm's requirements, call the algorithm, and provide either optimized results in a standard format for postprocessing, or an error messages if the optimization did not complete successfully. The SLSQP algorithm, which is not a global optimizer, is provided to assess problem feasibility and provide reasonable upper and lower bounds on metrics being optimized. Global optimization algorithms to implement were chosen according to the following criteria.

- Ability to perform constrained optimization with inequality constraints
- Ability to optimize without specified Jacobian or Hessian functions
- · Ability to specify bounds on individual decision variables
- Ability to work on a variety of potentially non-convex and otherwise complex problems

6.1.1 Solutions to residential pv multiobjective

The solve times listed are in addition to the time required to set up the problem and solve for the maximum allowable metric values, which currently uses the SLSQP algorithm. This setup time is between 10 and 15 seconds.

Minimizing LCOE subject to a total investment amount of \$3 MM USD and GHG being at least 40.

Objective Function	GHG Constraint Value	Solve Time (s)
Value		
0.037567	41.699885	145
0.037547	41.632867	589
0.037712	41.969348	~ 2
None found	None found	•
	Value 0.037567 0.037547 0.037712	Value 0.037567 41.699885 0.037547 41.632867 0.037712 41.969348

Additional details for each solution are given below under the section for the corresponding algorithm.

6.2 Sequential Least Squares Programming

The Sequential Least Squares Programming algorithm uses a gradient search method to locate a possibly local optimum. [6]

EpsilonConstraintOptimizer.maximize_slsqp(self, metric, max_amount=None, total_amount=None, min_metric=None, statistic=np.mean, initial=None, tol=1e-8, maxiter=50, verbose=0)

Maximize the objective function using the fmin_slsqp algorithm.

Parameters

metric [str] Name of metric to maximize. No default.

max_amount [DataFrame] Maximum investment amounts by R&D category (defined in investments data) and maximum metric values. Defaults to None.

total_amount [float] Upper limit on total investments summed across all R&D categories. Defaults to None.

min_metric [DataFrame] Lower limits on all metrics. Defaults to None.

statistic [function] Summary statistic used on the sample evaluations; the metric measure that is fed to the optimizer. Defaults to np.mean such that the optimization is performed on the means of relevant metrics.

initial [array of float] Initial value of decision variable(s) fed to the optimizer. Defaults to None.

tol [float] Requested accuracy of the optimized solution. Defaults to 1E-08.

maxiter [int] Maximum number of iterations the optimizer is permitted to execute. Defaults to 50.

verbose [int] Amount of information provided by the wrapper as the optimization is performed. Defaults to 0.

Return

results [Optimum instance] Container for an exit_code and exit_message received from the differential_evolution call, a list of optimized amounts and a list of optimized metrics.

A complete list of parameters and options for the fmin_slsqp algorithm is available in the documentation. [3]

6.2.1 Defining Constraints

Constraints for fmin_slsqp are defined either as a single function that takes as input a vector of decision variable values and returns an array containing the value of all constraints in the problem simultaneously. Both equality and inequality constraints can be defined, although they must be as separate functions and are provided to the fmin_slsqp algorithm under separate arguments.

6.2.2 SLSQP Solution to residential_pv_multiobjective

Solve time: 1.5 s

Decision Variable	Optimized Value		
BoS R&D	1.25 E-04		
Inverter R&D	3.64 E-08		
Module R&D	3.00 E+06		

System Metric	Optimized Value		
GHG	41.97		
LCOE	0.038		
Labor	0.032		

6.3 Differential Evolution

Differential evolution is one type of evolutionary algorithm that iteratively improves on an initial population, or set of potential solutions. [5] Differential evolution is well-suited to searching large solution spaces with multiple local minima, but does not guarantee convergence to the global minimum.

```
EpsilonConstraintOptimizer.maximize_diffev(self, metric, max_amount=None, total_amount=None, min_metric=None, statistic=np.mean, strategy='best1bin', tol=1e-8, maxiter=50, init='latinhypercube', verbose=0)
```

Parameters

metric [str] Name of metric to maximize. No default value.

max_amount [DataFrame] Maximum investment amounts by R&D category (defined in investments data) and maximum metric values. Defaults to None.

total_amount [float] Upper limit on total investments summed across all R&D categories. Defaults to None.

min_metric [DataFrame] Lower limits on all metrics. Defaults to None.

statistic [function] Summary statistic used on the sample evaluations; the metric measure that is fed to the optimizer. Defaults to np.mean such that the optimization is performed on the means of relevant metrics.

strategy [str] Which differential evolution strategy to use. Defaults to 'best1bin'. See [2] for full list.

- **seed** [int] Sets the random seed for optimization by creating a new RandomState instance. Defaults to 2 for reproducible solutions. If a value is not provided, then differential_evolution will return slightly different solutions for the same optimization problem every time it is called.
- init [str or array-like] Type of population initialization. Defaults to 'latinhypercube'. Alternative initializations are 'random' (which does not guarantee good coverage of the solution space) or specifying every member of the initial population in an array of shape (popsize, len(variables)). The latter option is useful when the global minimum is known to be in a small portion of the solution space, and the initialization can seed the population in this area. However, this parameter is not analogous to specifying initial values for decision variables, as each candidate solution in the population must be unique for the algorithm to optimize correctly.
- tol [float] Relative tolerance for convergence, which provides an upper limit on the standard deviation of candidate solutions. When this upper limit is met, the optimization has converged. Defaults to 0.01. The convergence tolerance for this algorithm was loosened compared to the other algorithms to lessen the execution time and increase the changes of the algorithm converging. Tighter tolerances (lower values of tol) tended to prevent the algorithm converging.
- **maxiter** [int] Upper limit on generations of candidate solution evolution, which corresponds to the number of algorithm iterations. Each iteration involves many function evaluations as each solution in the population evolves. Defaults to 75.

verbose [int] Amount of information provided by the wrapper as the optimization is performed. Defaults to 0.differential_evolution has no analogous verbosity parameter

Returns

out [Optimum instance] Container for an exit_code and exit_message received from the differential_evolution call, a list of optimized amounts and a list of optimized metrics.

A complete list of parameters and options for the $differential_evolution$ algorithm is available in the documentation. [2]

6.3.1 Defining Constraints

Constraints for differential_evolution are defined by passing the same multi-valued function defined in max-imize_slsqp to the NonLinearConstraint method. [7]

6.3.2 Differential Evolution Solutions to residential_pv_multiobjective

Solution 1

- Seed = 2
- Solve time = 145 s

Decision Variable	Optimized Value		
BoS R&D	9.62 E+02		
Inverter R&D	5.33 E+02		
Module R&D	2.99 E+06		

System Metric	Optimized Value		
GHG	41.70		
LCOE	0.038		
Labor	-0.456		

Solution 2

- Seed = 1
- Solve time = 589

Decision Variable	Optimized Value		
BoS R&D	4.70 E+03		
Inverter R&D	3.71 E+02		
Module R&D	2.99 E+06		

System Metric	Optimized Value		
GHG	41.63		
LCOE	0.037		
Labor	-2.29		

6.4 Simplicial Homology Global Optimization

The Simplicial Homology Global Optimization (SHGO) algorithm applies simplicial homology to general non-linear, low-dimensional optimization problems. [4]

```
EpsilonConstraintOptimizer.maximize_shgo(self, metric, max_amount=None, total_amount=None, min_metric=None, statistic=np.mean, tol=1e-8, maxiter=50, sampling_method='simplicial', verbose=0)
```

Maximize the objective function using the shgo global optimization algorithm.

Parameters

metric [str] Name of metric to maximize. No default value.

max_amount [DataFrame] Maximum investment amounts by R&D category (defined in investments data) and maximum metric values. Defaults to None.

total_amount [float] Upper metric_limit on total investments summed across all R&D categories. Defaults to None.

min_metric [DataFrame] Lower limits on all metrics. Defaults to None.

statistic [function] Summary statistic used on the sample evaluations; the metric measure that is fed to the optimizer. Defaults to np.mean such that the optimization is performed on the means of relevant metrics.

tol [float] Objective function tolerance in stopping criterion. Defaults to 1E-08.

maxiter [int] Upper limit on algorithm iterations that can be performed. One iteration involves many function evaluations. Defaults to 50.

sampling_method [str] Allowable values are 'sobol and 'simplicial'. Simplicial is default, uses less memory, and guarantees convergence (theoretically). Sobol is faster, uses more memory and does not guarantee convergence. Per documentation, Sobol is better for "easier" problems. Defaults to 'simplicial'.

verbose [int] Verbosity level returned by this wrapper function. No analogous parameters are available for shgo. Defaults to 0 (no messages returned during execution).

Returns

out [Optimum instance]: Container for an exit_code and exit_message received from the shgo call, a list of optimized amounts and a list of optimized metrics.

shgo does not have a parameter that sets the initial decision variable values. A complete list of parameters available for the shgo algorithm is available in the documentation. [1]

6.4.1 Defining Constraints

Constraints for shoo must be provided as a dictionary or sequence of dictionaries with the following format:

Each of the constraint functions g1 (x), h1 (x), and so on are functions that take decision variable values as inputs and return the value of the constraint. Inequality constraints (g1 (x) and g2 (x) above) are formulated as $g(x) \ge 0$ and equality constraints (h1 (x) and h2 (x) above) are formulated as h(x) = 0. Each constraint in the optimization problem is defined as a separate function, with a separate dictionary giving the constraint type. With shgo it is not possible to use one function that returns a vector of constraint values.

6.5 References

- scipy.optimize.shgoSciPyv1.5.4 Reference Guide: Optimization and root finding (scipy.optimize)
 URL: https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.shgo.html#rb2e152d227b3-1 Last accessed 12/28/2020.
- 2. scipy.optimize.differential_evolution SciPy v1.5.4 Reference Guide: Optimization and root finding (scipy.optimize) URL: https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize. differential_evolution.html Last accessed 12/28/2020.
- 3. scipy.optimize.fmin_slsqp SciPy v1.5.4 Reference Guide: Optimization and root finding (scipy.optimize) URL: https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.fmin_slsqp.html Last accessed 12/28/2020.
- 4. Endres, SC, Sandrock, C, Focke, WW. (2018) "A simplicial homology algorithm for Lipschitz optimisation", Journal of Global Optimization (72): 181-217. URL: https://link.springer.com/article/10.1007/s10898-018-0645-y
- 5. Storn, R and Price, K. (1997) "Differential Evolution a Simple and Efficient Heuristic for Global Optimization over Continuous Spaces", Journal of Global Optimization (11): 341 359. URL: https://link.springer.com/article/10.1023/A:1008202821328
- 6. Kraft D (1988) A software package for sequential quadratic programming. Tech. Rep. DFVLR-FB 88-28, DLR German Aerospace Center Institute for Flight Mechanics, Koln, Germany.
- 7. scipy.optimize.NonlinearConstraint SciPy v1.5.4 Reference Guide: Optimization and root finding (scipy.optimize) URL: https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize. NonlinearConstraint.html Last accessed 12/29/2020.

USER INTERFACE

The Eutychia interface is a user's portal to interact with the Tyche decision support tool. Users can make decisions to change investments and the metrics by which they will be assessed (as described in the following sections). Eutychia aims to aide in formalizing funding processes to make technically and analytically-based decisions, through modeling possible scenarios and generating visualizations to communicate these results. Tool output aims to aide decision-makers in

- 1. **Focused analysis** comparing investment scenarios to examine impact across metrics when exploring options during the decision-making process and
- Broader communication of Office goals externally, such as through the dissemination of a funding opportunity announcement.

Feedback is appreciated to enhance the interface to best meet user needs.

7.1 User Input

Investment Categories A user can suggest research foci by selecting **investment categories** and **investment levels** (\$) in each topic area and/or across the investment portfolio. In the current iteration of the Eutychia prototype, users have the option to select a budget for each of the following investment categories: 1. Balance of System R&D 1. Inverter R&D 1. Module R&D

Later-stage iterations of the prototype will include as many categories as the user selects for which data is available.

Metrics A user can also select up to three metrics to impact through R&D on these selected investment categories and specify goals that must be met. The current options include: 1. Greenhouse gas emissions ($\Delta gCO2e/system$) 1. Labor ($\Delta :math:/system$) 1. Levelized cost of energy (Δ /kWh)

7.2 Modes

The Eutychia interface operates in two modes: 1. **Explore Mode**, checked by default, 1. **Optimize Mode**, which can be enabled by deselecting "explore." Entering Optimize Mode allows users to update optimization parameters.

The selected mode determines which user inputs can be edited. The following table summarizes the parameters that can be updated, the corresponding optimizer parameter name, and the widget (currently) used to make this change.

	Parameter	Widget	Explore Mode	Optimize Mode
Investment level (USD) by category	max_amount	slider	X	X
Total portfolio investment (USD)	total_amount	slider		X
Metric constraint	min_metric	slider		X
Optimization metric to maximize	metric	dropdown		X

In either mode, changes made to investment level(s) by category will be reflected immediately in the output visualizations. In Optimize Mode, once satisfied with the selected metrics, the user can click "optimize" to model the chosen scenario.

7.3 Visualizations

Users are presented with the option to interact with the data in varying levels of detail. These options are enabled to suit the needs of users, from those who prefer a snapshot of the bigger picture for quick analysis to those who would like to study the distributional probability of achieving each metric. Plots are generated using the Seaborn 0.11.0 package. The available visualizations in order of increasing level of detail include:

- 1. **Heatmaps** (heatmap) with metric scaled to percent of the maximum possible improvement,
- 2. Annotated heatmaps with metric values overlayed, and
- 3. **Distributions** with the probability of ahieving each metric based on the number of samples. At this stage of development, these results can be viewed in columns (by metric) or in a grid. The user can select from the following options:
 - Box plots (boxplot)
 - Probability distributions (kdeplot)
 - Violin plots (violinplot)

A user can toggle between their visualization options using the links (heatmap, column, grid) at the top left-hand corner of the screen. By default, Eutychia opens to the grid layout.

7.4 References

¹ Michael Waskom, Olga Botvinnik, Maoz Gelbart, Joel Ostblom, Paul Hobson, Saulius Lukauskas, David C Gemperline, et al. 2020. Mwaskom/Seaborn: V0.11.0 (Sepetmber 2020). Zenodo. https://doi.org/10.5281/zenodo.4019146.

CHAPTER

EIGHT

TUTORIAL

Multiple Objectives for Residential PV.

8.1 Import packages.

```
import os
import sys
sys.path.insert(0, os.path.abspath("../src"))
```

8.2 Load data.

The data are stored in a set of tab-separated value files in a folder.

```
designs = ty.Designs("../data/residential_pv_multiobjective")
```

```
investments = ty.Investments("../data/residential_pv_multiobjective")
```

Compile the production and metric functions for each technology in the dataset.

```
designs.compile()
```

8.3 Examine the data.

The functions table specifies where the Python code for each technology resides.

designs.functions

Right now, only the style numpy is supported.

The indices table defines the subscripts for variables.

designs.indices

The designs table contains the cost, input, efficiency, and price data for a scenario.

designs.designs

The parameters table contains additional techno-economic parameters for each technology.

designs.parameters

The results table specifies the units of measure for results of computations.

designs.results

The tranches table specifies multually exclusive possibilities for investments: only one Tranch may be selected for each Category.

investments.tranches

The investments table bundles a consistent set of tranches (one per category) into an overall investment.

investments.investments

8.4 Evaluate the scenarios in the dataset.

scenario_results = designs.evaluate_scenarios(sample_count=50)

scenario_results.xs(1, level="Sample", drop_level=False)

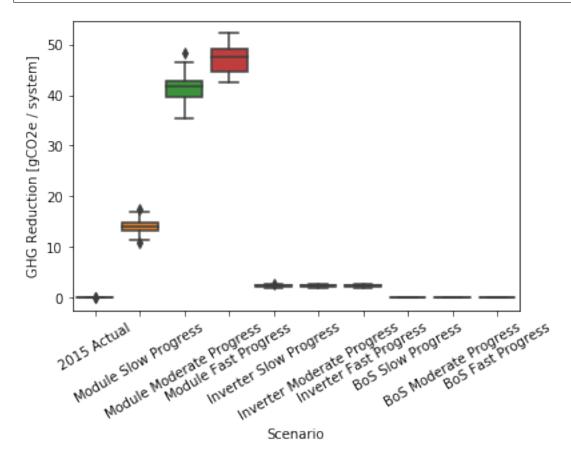
8.4.1 Save results.

scenario_results.to_csv("output/residential_pv_multiobjective/example-scenario.csv")

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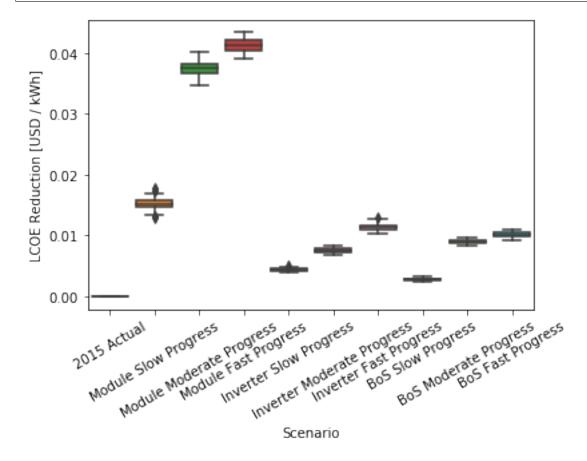
8.4.2 Plot GHG metric.

```
g = sb.boxplot(
   x="Scenario",
   y="Value",
    data=scenario_results.xs(
        ["Metric", "GHG"],
        level=["Variable", "Index"]
   ).reset_index()[["Scenario", "Value"]],
   order=[
        "2015 Actual"
        "Module Slow Progress"
        "Module Moderate Progress"
        "Module Fast Progress"
        "Inverter Slow Progress"
        "Inverter Moderate Progress"
        "Inverter Fast Progress"
        "BoS Slow Progress"
        "BoS Moderate Progress"
        "BoS Fast Progress"
    ]
g.set(ylabel="GHG Reduction [gCO2e / system]")
g.set_xticklabels(g.get_xticklabels(), rotation=30);
```



8.4.3 Plot LCOE metric.

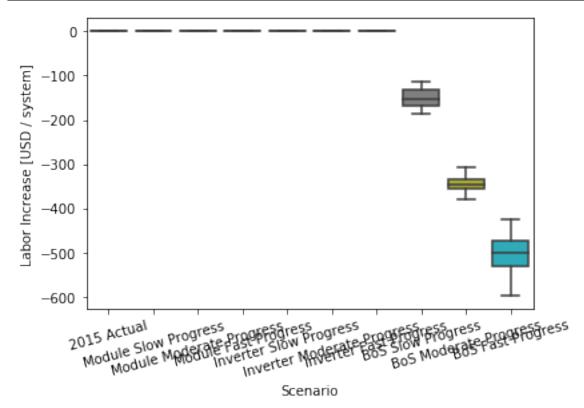
```
g = sb.boxplot(
   x="Scenario",
   y="Value",
   data=scenario_results.xs(
        ["Metric", "LCOE"],
        level=["Variable", "Index"]
   ).reset_index()[["Scenario", "Value"]],
   order=[
        "2015 Actual"
        "Module Slow Progress"
        "Module Moderate Progress"
        "Module Fast Progress"
        "Inverter Slow Progress"
        "Inverter Moderate Progress"
        "Inverter Fast Progress"
        "BoS Slow Progress"
        "BoS Moderate Progress"
        "BoS Fast Progress"
    ]
g.set(ylabel="LCOE Reduction [USD / kWh]")
g.set_xticklabels(g.get_xticklabels(), rotation=30);
```



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8.4.4 Plot labor metric.

```
g = sb.boxplot(
   x="Scenario",
   y="Value",
   data=scenario_results.xs(
        ["Metric", "Labor"],
        level=["Variable", "Index"]
   ).reset_index()[["Scenario", "Value"]],
   order=[
        "2015 Actual"
        "Module Slow Progress"
        "Module Moderate Progress"
        "Module Fast Progress"
        "Inverter Slow Progress"
        "Inverter Moderate Progress"
        "Inverter Fast Progress"
        "BoS Slow Progress"
        "BoS Moderate Progress"
        "BoS Fast Progress"
    ]
g.set(ylabel="Labor Increase [USD / system]")
g.set_xticklabels(g.get_xticklabels(), rotation=15);
```



8.5 Evaluate the investments in the dataset.

```
investment_results = investments.evaluate_investments(designs, sample_count=50)
```

8.5.1 Costs of investments.

```
investment_results.amounts
```

8.5.2 Benefits of investments.

```
investment_results.metrics.xs(1, level="Sample", drop_level=False)
```

```
investment_results.summary.xs(1, level="Sample", drop_level=False)
```

8.5.3 Save results.

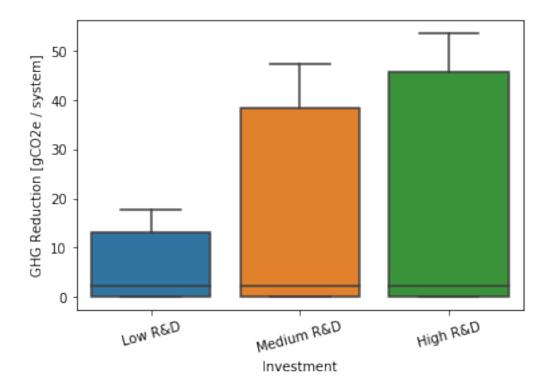
```
investment_results.amounts.to_csv("output/residential_pv_multiobjective/example-
investment-amounts.csv")
```

```
investment_results.metrics.to_csv("output/residential_pv_multiobjective/example-
investment-metrics.csv")
```

8.5.4 Plot GHG metric.

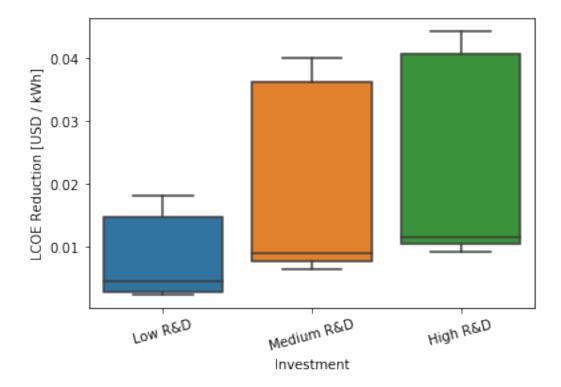
```
g = sb.boxplot(
    x="Investment",
    y="Value",
    data=investment_results.metrics.xs(
        "GHG",
        level="Index"
    ).reset_index()[["Investment", "Value"]],
    order=[
        "Low R&D" ,
        "Medium R&D",
        "High R&D" ,
    ]
)
g.set(ylabel="GHG Reduction [gCO2e / system]")
g.set_xticklabels(g.get_xticklabels(), rotation=15);
```

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8.5.5 Plot LCOE metric.

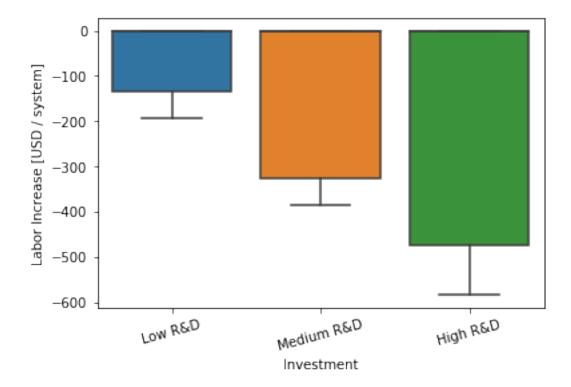
```
g = sb.boxplot(
    x="Investment",
    y="Value",
    data=investment_results.metrics.xs(
        "LCOE",
        level="Index"
    ).reset_index()[["Investment", "Value"]],
    order=[
        "Low R&D"
        "Medium R&D",
        "High R&D" ,
        ]
)
g.set(ylabel="LCOE Reduction [USD / kWh]")
g.set_xticklabels(g.get_xticklabels(), rotation=15);
```



8.5.6 Plot labor metric.

```
g = sb.boxplot(
    x="Investment",
    y="Value",
    data=investment_results.metrics.xs(
        "Labor",
        level="Index"
    ).reset_index()[["Investment", "Value"]],
    order=[
        "Low R&D" ,
        "Medium R&D",
        "High R&D" ,
        ]
)
g.set(ylabel="Labor Increase [USD / system]")
g.set_xticklabels(g.get_xticklabels(), rotation=15);
```

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8.6 Multi-objective decision analysis.

8.6.1 Compute costs and metrics for tranches.

Tranches are atomic units for building investment portfolios. Evaluate all of the tranches, so we can assemble them into investments (portfolios).

```
tranche_results = investments.evaluate_tranches(designs, sample_count=50)
```

Display the cost of each tranche.

```
tranche_results.amounts
```

Display the metrics for each tranche.

```
tranche_results.summary
```

Save the results.

8.6.2 Fit a response surface to the results.

The response surface interpolates between the discrete set of cases provided in the expert elicitation. This allows us to study funding levels intermediate between those scenarios.

```
evaluator = ty.Evaluator(investments.tranches, tranche_results.summary)
```

Here are the categories of investment and the maximum amount that could be invested in each:

```
evaluator.max_amount
```

Here are the metrics and their units of measure:

```
evaluator.units
```

Example interpolation.

Let's evaluate the case where each category is invested in at half of its maximum amount.

```
example_investments = evaluator.max_amount / 2
example_investments
```

```
evaluator.evaluate(example_investments)
```

```
Category
           Index Sample
BoS R&D
           GHG
                            -0.0010586097518157094
                  1
                             7.493162517135921e-05
                  3
                              0.001253893601450784
                              -0.00398626797827717
                             -0.005572343870333896
Module R&D Labor 46
                            0.014371009324918305
                  47
                             0.011128728287076228
                  48
                             0.0039832773605894545
                  49
                             0.006026680267950724
                  50
                              0.028844695933457842
Name: Value, Length: 450, dtype: object
```

Let's evaluate the mean instead of outputing the whole distribution.

```
evaluator.evaluate_statistic(example_investments, np.mean)
```

```
Index
GHG 30.156830
LCOE 0.038160
Labor -246.843027
Name: Value, dtype: float64
```

Here is the standard deviation:

```
evaluator.evaluate_statistic(example_investments, np.std)
```

```
Index
GHG 1.410956
```

(continues on next page)

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```
LCOE 0.000850
Labor 16.070395
Name: Value, dtype: float64
```

A risk-averse decision maker might be interested in the 10% percentile:

```
evaluator.evaluate_statistic(example_investments, lambda x: np.quantile(x, 0.1))
```

```
Index
GHG 28.573627
LCOE 0.037140
Labor -268.059699
Name: Value, dtype: float64
```

8.6.3 ε-Constraint multiobjective optimization

```
optimizer = ty.EpsilonConstraintOptimizer(evaluator)
```

In order to meaningfully map the decision space, we need to know the maximum values for each of the metrics.

```
metric_max = optimizer.max_metrics()
metric_max
```

```
GHG 49.429976

LCOE 0.062818

Labor 0.049555

Name: Value, dtype: float64
```

Example optimization.

Limit spending to \$3M.

```
investment_max = 3e6
```

Require that the GHG reduction be at least 40 gCO2e/system and that the Labor wages not decrease.

```
metric_min = pd.Series([40, 0], name = "Value", index = ["GHG", "Labor"])
metric_min
```

```
GHG 40
Labor 0
Name: Value, dtype: int64
```

Compute the ε -constrained maximum for the LCOE.

```
'Optimization terminated successfully.'
```

Here are the optimal spending levels:

```
np.round(optimum.amounts)
```

```
Category
BoS R&D 0.0
Inverter R&D 0.0
Module R&D 3000000.0
Name: Amount, dtype: float64
```

Here are the three metrics at that optimum:

```
optimum.metrics
```

```
Index
GHG 41.627691
LCOE 0.037566
Labor 0.028691
Name: Value, dtype: float64
```

Thus, by putting all of the investment into Module R&D, we can expected to achieve a mean 3.75 ¢/kWh reduction in LCOE under the GHG and Labor constraints.

It turns out that there is no solution for these constraints if we evaluate the 10th percentile of the metrics, for a risk-averse decision maker.

```
'Iteration limit exceeded'
```

Let's try again, but with a less stringent set of constraints, only constraining GHG somewhat but not Labor at all.

```
optimum = optimizer.maximize(
    "LCOE"
    total_amount = investment_max
    min_metric = pd.Series([30], name = "Value", index = ["GHG"]),
    statistic = lambda x: np.quantile(x, 0.1)
)
optimum.exit_message
```

```
'Optimization terminated successfully.'
```

```
np.round(optimum.amounts)
```

```
Category
BoS R&D 0.0
Inverter R&D 0.0
```

(continues on next page)

(continued from previous page)

```
Module R&D 3000000.0
Name: Amount, dtype: float64
```

```
optimum.metrics
```

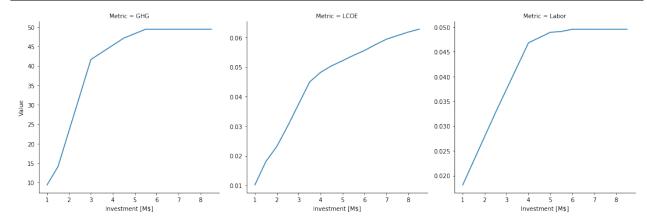
```
Index
GHG 39.046988
LCOE 0.036463
Labor -0.019725
Name: Value, dtype: float64
```

8.6.4 Pareto surfaces.

Metrics constrained by total investment.

```
pareto_amounts = None
for investment_max in np.arange(1e6, 9e6, 0.5e6):
    metrics = optimizer.max_metrics(total_amount = investment_max)
    pareto_amounts = pd.DataFrame(
        [metrics.values]
        columns = metrics.index.values
        index = pd.Index([investment_max / 1e6], name = "Investment [M$]"),
    ).append(pareto_amounts)
pareto_amounts
```

```
<seaborn.axisgrid.FacetGrid at 0x7f9da11752b0>
```



We see that the LCOE metric saturates more slowly than the GHG and Labor ones.

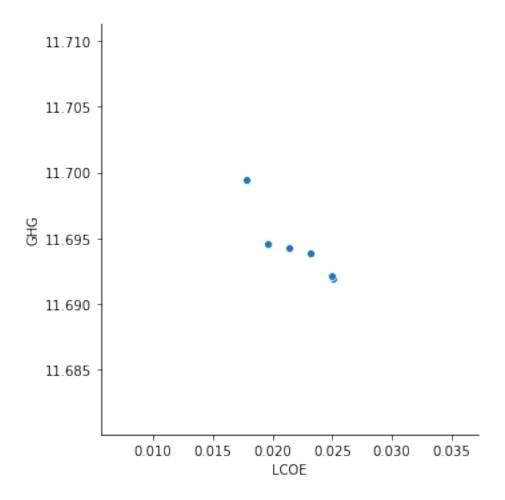
GHG vs LCOE, constrained by total investment.

```
investment_max = 3
pareto_ghg_lcoe = None
for lcoe_min in 0.95 * np.arange(0.5, 0.9, 0.05) * pareto_amounts.loc[investment_max,
→"LCOE"]:
   optimum = optimizer.maximize(
       "GHG",
       max_amount
                   = pd.Series([0.9e6, 3.0e6, 1.0e6], name = "Amount", index = [
→"BoS R&D", "Inverter R&D", "Module R&D"]),
       total_amount = investment_max * 1e6
       min_metric = pd.Series([lcoe_min], name = "Value", index = ["LCOE"]),
   pareto_ghg_lcoe = pd.DataFrame(
       [[investment_max, lcoe_min, optimum.metrics["LCOE"], optimum.metrics["GHG"],__
→optimum.exit_message]],
       columns = ["Investment [M$]", "LCOE (min)", "LCOE", "GHG", "Result"]
   ).append(pareto_ghg_lcoe)
pareto_ghg_lcoe = pareto_ghg_lcoe.set_index(["Investment [M$]", "LCOE (min)"])
pareto_ghg_lcoe
```

```
sb.relplot(
    x = "LCOE",
    y = "GHG",
    kind = "scatter",
    data = pareto_ghg_lcoe#[pareto_ghg_lcoe.Result == "Optimization terminated_
    successfully."]
)
```

```
<seaborn.axisgrid.FacetGrid at 0x7f9da13ae630>
```

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The three types of investment are too decoupled to make an interesting pareto frontier, and we also need a better solver if we want to push to lower right.

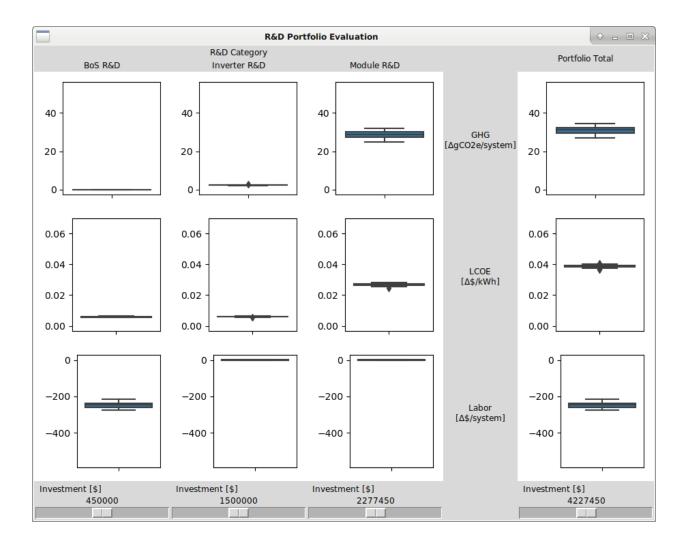
8.7 Run the interactive explorer for the decision space.

Make sure the the tk package is installed on your machine. Here is the Anaconda link: https://anaconda.org/anaconda/tk.

```
w = ty.DecisionWindow(evaluator)
w.mainloop()
```

A new window should open that looks like the image below. Moving the sliders will cause a recomputation of the boxplots.

```
Image("residential_pv_multiobjective_gui.png")
```



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CHAPTER

NINE

MOCK FOA

9.1 Background

Understanding the FOA process is essential to designing an effective tool to make to make technically and analytically-based decisions. The "Mock FOA" process takes a service design approach to understanding the FOA-writing process as it stands. The Mock FOA began with interviews with five previous DOE detailees and seven senior DOE staff who have led multiple FOA development efforts. A major theme emerged: effective communication of analysis logic and results poses one of the largest challenges during the FOA process.

A decision-support tool could assist in the communication necessary to percolate this technical information up the chain. Interview findings were formalized in collaboration with the NREL service design team to understand where such a tool could make the greatest impact. The team considered the steps taken to issue a FOA, resources referenced, and decision-makers involved.

9.1.1 Phases

Interviews revealed that, while all FOA processes are unique and highly non-linear, specific actions must occur. These characterize phases of the FOA journey:

- 1. Launch. Decide to issue a FOA.
- 2. Frame. Formulate a plan to collect the information necessary to write the FOA
- 3. **Scope**. Investigate topic options.
- 4. **Draft**. Compile information into draft FOA.
- 5. **Refine**. Prepare FOA for distribution.

The specific needs of each phase inform the tool **content**.

9.1.2 Roles

The team considered that different staff members will interact with this information differently and prefer different methods of data communication. These roles were characterized by "personae" defined by level of involvement in the FOA-writing process.

- · Technical analyst
- · Technical lead
- FOA lead
- Approver

Decision makers in each of these roles will interact with tool output. The tool users determine how the tool will be used and how its content will be displayed, informing **interactions and data visualization**. For example, a user who will view the tool output in a presentation will need a static representation of the tool output.

9.2 Potential topics

Prototyping a tool requires content. The team referenced two previous FOAs to understand the break-down of topic areas. We then extracted FOA topic/subtopic areas and metrics from 2016 budget request, combining hard/soft cost-focused FOAs to examine how to compete the two and avoid directly analyzing a specific past FOA. Following this process further informed the team's understanding of how decision-makers might decide what to input into the tool.

Topics under consideration might be assessed by the following metrics:

- \$/W_{DC}
- \$/kWh
- Strategic metal content (lifetime)
- Hazardous waste content (lifetime)
- Lifetime
- · Reliability
- · Emissions
- Labor

The following text details topic areas considered for Tyche tool development.

9.2.1 1. Crystaline silicon wafer design

- · Wafer area
- · Wafer thickness
- · Wafer density
- · Silicon utilization
- · Production yield

9.2.2 2. Tandem thin-films

- Design parameters
- · Architectures

9.2.3 3. Polysilicon module

• (many parameters)

9.2.4 4. Module design

- Module Capital
- Module Lifetime
- Module Efficiency
- Module Aperture
- Module O&M Fixed
- Module Degradation
- Module Soiling Loss

9.2.5 5. Inverter design

- Inverter Capital
- Inverter Lifetime
- Inverter Replacement
- Inverter Efficiency

9.2.6 6. Balance-of-system design

- · Hardware Capital
- Direct Labor
- Permitting
- Customer Acquisition
- Installer Overhead & Profit

9.2. Potential topics

DEPLOYMENT PLAN

10.1 Objectives

- 1. Securely house all potentially sensitive data within on DOE servers within the DOE intranet.
- 2. Minimize the deployment and maintenance burden at DOE.
- 3. Assure the quality of software and data updates.
- 4. Enable DOE personnel and contractors to contribute technology models and data.

10.2 Components and Activities

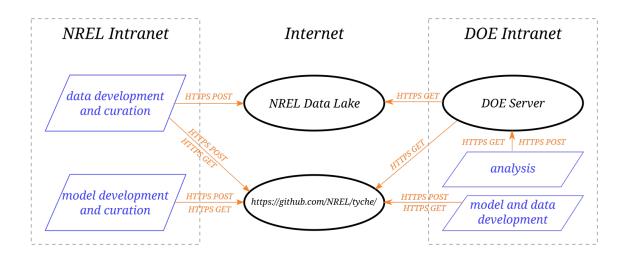


Fig. 10.1: Deployment of services and activities.

10.3 Activities

Analysts at DOE will connect to Tyche server within the DOE intranet using their web browsers to run and analyze scenarios using Tyche. The server will have the capability to record scenarios for sharing within DOE, but that data will never leave the DOE intranet.

Analysts developing data and technology models at DOE, NREL, and elsewhere can post that data and software to a branch of the GitHub Software Repository. Those contributions will be reviewed, vetted, and tested before they are pushed to the NREL Data Lake (in the case of datasets) or to the production branch of the GitHub repository (in the case of technology models).

NREL will perform quality assurance and periodically update the production version of the data and software, both of which can be fetched by DOE on a regular basis.

10.4 Components

10.4.1 DOE Server

The DOE server for Tyche resides within the DOE intranet. It fetches software updates from the GitHub Software Repository and fetches data updates from the NREL Data Lake. (Because data volumes are small, it could perform these automatically on a daily or weekly basis during off hours.) It runs a Quart HTTP server within a Conda environment. Requirements for this server are as follows:

- 1. Linux (preferred) or Windows.
- 2. Four to 16 CPU cores and at least 32 GB of memory.
- 3. An up-to-date installation (version 4.8.3 or later) of the Conda software package manager.
- 4. Installation of the Tyche environment within Conda. (This will install the correct version of Python and the other required software, so those need not be installed individually.) See the attachment conda-environment.yml.
- 5. Running a shell script for the Quart HTTP server.
- 6. Open outgoing HTTPS ports for GET requests to the NREL Data Lake and GitHub.com.
- 7. An open HTTP incoming port from client web browsers withing the DOE intranet.
- 8. A folder on disk that is regularly backed up.

10.4.2 NREL Data Lake

The NREL Data Lake, which is housed on Amazon Web Services (AWS), contains all of the non-sensitive data, such as the parameters for technology models and the results of expert elicitations. NREL curates the data that is pushed to the data lake.

10.4.3 GitHub Software Repository

The Tyche software resides on the NREL GitHub software repository https://github.com/NREL/tyche/. The production branch contains the latest deployable version of the software. Other branches contain work in progress, contributions from DOE and its subcontractors, and the development (pre-release) version of the software.

10.5 Security Considerations

- 1. NREL has authority to operate (ATO) with non-sensitive software and data on its Data Lake and on GitHub.com.
- 2. Sensitive data (in the form of scenario definitions and results) may reside on the DOE server and on the laptops of DOE users.
- 3. The Tyche service only makes HTTPS GET requests outside of the DOE intranet, and these only consist of fetching non-sensitive datasets and technology models. Thus, the firewall for the Tyche server should be configured at follows:
 - 1. Block all incoming traffic from outside the DOE intranet.
 - 2. Allow incoming HTTP traffic from inside the DOE intranet.
 - 3. Allow outgoing HTTPS traffic to NREL Data Lake and GitHub.com.
 - 4. Block all other outgoing traffic.
- 4. Ideally, the Tyche software (and its library dependencies) and its updates should undergo a security audit.

CHAPTER

ELEVEN

GETTING STARTED

Instruction for Running the Example and the Server

11.1 Conda Environment

Before running the example or the server, create and activate the conda environment:

```
conda env create --file conda/win.yml
conda activate tyche
```

on Windows, or on Mac

```
conda env create --file conda/mac.yml conda activate tyche
```

Note that the conda environment was created with the command:

conda create -n tyche -c conda-forge python=3.7 numpy scipy scikit-learn seaborn=0.10 $_{-}$ \rightarrow matplotlib=3.3 quart hypercorn jupyter

11.2 Running the Server

Start the server in debug mode

on Windows, or on Mac

debug.cmd

./debug.sh

or in production mode

run.cmd

on Windows, or on Mac

./run.sh

and then visit http://127.0.0.1:5000/.

11.3 Running the Example

Using Jupyter, first start the notebook server

jupyter notebook

and visit http://localhost:8888/ to select example.ipynb.

Alternatively, just open example.py is the IDE of your choice or run it at the command line.

CHAPTER

TWELVE

PYTHON API

The tyche module is a Python package for R&D pathways analysis and evaluation. It contains five Python classes for R&D pathway decision support.

- Designs for specifying and evaluating technology decisions in the presence of uncertainty.
- Investments for specifying and evaluating R&D portfolios consisting of multiple technology-investment options.
- Evaluator for rapidly evaluating the costs and benefits for sets of portfolios.
- EpsilonConstraints for multi-objective optimization using a generalization of the epsilon-constraint technique.
- DecisionGUI for interactively exploring the costs and benefits of R&D portfolios.

12.1 tyche package

12.1.1 Submodules

12.1.2 tyche.DecisionGUI module

Interactive exploration of a technology.

```
class tyche.DecisionGUI.DecisionWindow(evaluator)
    Bases: object
```

Class for displaying an interactive interface to explore cost-benefit tradeoffs for a technology.

```
{\tt create\_figure}\,(i,j) \, 	o \, {\tt matplotlib.figure.Figure}
```

Run the interactive interface.

reevaluate (next=<function DecisionWindow.<lambda>>, delay=200)

Recalculate the results after a delay.

Parameters

- **next** (function) The operation to perform after completing the recalculation.
- **delay** (*int*) The number of milliseconds to delay before the recalculation.

reevaluate_immediate (next=<function DecisionWindow.<lambda>>)

Recalculate the results immediately.

Parameters next (function) – The operation to perform after completing the recalculation.

```
refresh()
          Refresh the graphics after a delay.
     refresh_immediate()
          Refresh the graphics immediately.
12.1.3 tyche.Designs module
Designs for technologies.
class tyche.Designs.Designs(path=None,
                                                   indices='indices.tsv',
                                                                       functions='functions.tsv',
                                     signs='designs.tsv', parameters='parameters.tsv', results='results.tsv')
     Bases: object
     Designs for a technology.
     indices
          The indices table.
              Type DataFrame
     functions
          The functions table.
              Type DataFrame
     designs
          The designs table.
              Type DataFrame
     parameters
          The parameters table.
              Type DataFrame
     results
          The results table.
              Type DataFrame
     compile()
          Compile the production and metrics functions.
     evaluate (technology, sample_count=1)
          Evaluate the performance of a technology.
              Parameters
                  • technology (str) – The name of the technology.
                  • sample_count (int) – The number of random samples.
     evaluate_scenarios (sample_count=1)
          Evaluate scenarios.
              Parameters sample_count (int) - The number of random samples.
     vectorize_designs (technology, scenario_count, sample_count=1)
          Make an array of designs.
     vectorize_indices (technology)
```

Make an array of indices.

- **x** (array) The array.
- sample_count (int) The sample size.

12.1.4 tyche.Distributions module

Utilities for probability distributions.

```
tyche. Distributions. choice (a, size=None, replace=True, p=None)

Generates a random sample from a given 1-D array
```

New in version 1.7.0.

Note: New code should use the choice method of a default_rng() instance instead; see *random-quick-start*.

Parameters

- **a** (1-D array-like or int) If an ndarray, a random sample is generated from its elements. If an int, the random sample is generated as if a were np.arange(a)
- size (int or tuple of ints, optional) Output shape. If the given shape is, e.g., (m, n, k), then m * n * k samples are drawn. Default is None, in which case a single value is returned.
- replace (boolean, optional) Whether the sample is with or without replacement
- **p** (1-D array-like, optional) The probabilities associated with each entry in a. If not given the sample assumes a uniform distribution over all entries in a.

Returns samples – The generated random samples

Return type single item or ndarray

Raises ValueError – If a is an int and less than zero, if a or p are not 1-dimensional, if a is an array-like of size 0, if p is not a vector of probabilities, if a and p have different lengths, or if replace=False and the sample size is greater than the population size

See also:

```
randint(), shuffle(), permutation()
```

Generator.choice() which should be used in new code

Examples

Generate a uniform random sample from np.arange(5) of size 3:

```
>>> np.random.choice(5, 3)
array([0, 3, 4]) # random
>>> #This is equivalent to np.random.randint(0,5,3)
```

Generate a non-uniform random sample from np.arange(5) of size 3:

```
>>> np.random.choice(5, 3, p=[0.1, 0, 0.3, 0.6, 0])
array([3, 3, 0]) # random
```

Generate a uniform random sample from np.arange(5) of size 3 without replacement:

```
>>> np.random.choice(5, 3, replace=False)
array([3,1,0]) # random
>>> #This is equivalent to np.random.permutation(np.arange(5))[:3]
```

Generate a non-uniform random sample from np.arange(5) of size 3 without replacement:

```
>>> np.random.choice(5, 3, replace=False, p=[0.1, 0, 0.3, 0.6, 0])
array([2, 3, 0]) # random
```

Any of the above can be repeated with an arbitrary array-like instead of just integers. For instance:

tyche.Distributions.constant(value)

The constant distribution.

Parameters value (float) – The constant value.

tyche.Distributions.mixture(weights, distributions)

A mixture of two distributions.

Parameters

- weights (array of float) The weights of the distributions to be mixed.
- distributions (array of distributions) The distributions to be mixed.

tyche.Distributions.parse_distribution(text)

Make the Python object for the distribution, if any is specified.

Parameters text (str) – The Python expression for the distribution, or plain text.

12.1.5 tyche.EpsilonConstraints module

Epsilon-constraint optimization.

Bases: object

An epsilon-constration multi-objective optimizer.

evaluator

The technology evaluator.

Type tyche. Evaluator

scale

The scaling factor for output.

Type float

max_metrics (max_amount=None, total_amount=None, statistic=<function mean>, tol=1e-08, maxiter=50, verbose=0)

Maximum value of metrics. @todo update to include additional algorithms :param max_amount: The maximum amounts that can be invested in each category. :type max_amount: DataFrame :param total_amount: The maximum amount that can be invested *in toto*. :type total_amount: float :param min_metric: The minimum constraint for each metric. :type min_metric: DataFrame :param statistic: The statistic used on the sample evaluations. :type statistic: function :param initial: The initial value for the search. :type initial: array of float :param tol: The search tolerance. :type tol: float :param maxiter: The maximum iterations for the search. :type maxiter: int :param verbose: Verbosity level. :type verbose: int

maximize_diffev (metric, max_amount=None, total_amount=None, min_metric=None, statistic=<function mean>, strategy='best1bin', seed=2, tol=0.01, maxiter=75, init='latinhypercube', verbose=0)

Maximize the objective function using the differential_evoluation algorithm.

Parameters

- **metric** (str) Name of metric to maximize.
- max_amount (DataFrame) Maximum investment amounts by R&D category (defined in investments data) and maximum metric values
- total_amount (float) Upper limit on total investments summed across all R&D categories.
- min_metric (DataFrame) Lower limits on all metrics.
- **statistic** (*function*) Summary statistic used on the sample evaluations; the metric measure that is fed to the optimizer.
- **strategy** (*str*) Which differential evolution strategy to use. 'best1bin' is the default. See algorithm docs for full list.
- **seed** (*int*) Sets the random seed for optimization by creating a new *RandomState* instance. Defaults to 1. Not setting this parameter means the solutions will not be reproducible.
- **init** (str or array-like) Type of population initialization. Default is Latin hypercube; alternatives are 'random' or specifying every member of the initial population in an array of shape (popsize, len(variables)).
- tol (float) Relative tolerance for convergence
- maxiter (int) Upper limit on generations of evolution (analogous to algorithm iterations)

- **verbose** (*int*) Verbosity level returned by this outer function. differential_evolution has no verbosity parameter
- maximize_shgo (metric, max_amount=None, total_amount=None, min_metric=None, statistic=<function mean>, tol=1e-08, maxiter=50, sampling_method='simplicial', verbose=0)

Maximize the objective function using the shgo global optimization algorithm.

Parameters

- **metric** (str) Name of metric to maximize.
- max_amount (DataFrame) Maximum investment amounts by R&D category (defined in investments data) and maximum metric values
- total_amount (float) Upper metric_limit on total investments summed across all R&D categories.
- min_metric (DataFrame) Lower limits on all metrics.
- **statistic** (function) Summary metric_statistic used on the sample evaluations; the metric measure that is fed to the optimizer.
- tol (float) Objective function tolerance in stopping criterion.
- maxiter (int) Upper metric limit on iterations that can be performed
- **sampling_method** (*str*) Allowable values are 'sobol and 'simplicial'. Simplicial is default, uses less memory, and guarantees convergence (theoretically). Sobol is faster, uses more memory and does not guarantee convergence. Per documentation, Sobol is better for "easier" problems.
- **verbose** (*int*) Verbosity level returned by this outer function.

maximize_slsqp (metric, max_amount=None, total_amount=None, min_metric=None, statistic=<function mean>, initial=None, tol=1e-08, maxiter=50, verbose=0)

Maximize the objective function using the fmin slsqp algorithm.

Parameters

- metric (str) Name of metric to maximize.
- max_amount (DataFrame) Maximum investment amounts by R&D category (defined in investments data) and maximum metric values
- total_amount (float) Upper limit on total investments summed across all R&D categories.
- min metric (DataFrame) Lower limits on all metrics.
- **statistic** (function) Summary statistic used on the sample evaluations; the metric measure that is fed to the optimizer.
- initial (array of float) Initial value of decision variable(s) fed to the optimizer.
- **tol** (*float*) Search tolerance fed to the optimizer.
- maxiter (int) Maximum number of iterations the optimizer is permitted to execute.
- **verbose** (*int*) Verbosity level returned by the optimizer and this outer function.

class tyche.EpsilonConstraints.Optimum (exit_code, exit_message, amounts, metrics)
 Bases: tuple

Named tuple type for optimization results.

property amounts

Alias for field number 2

property exit_code

Alias for field number 0

property exit_message

Alias for field number 1

property metrics

Alias for field number 3

12.1.6 tyche. Evaluator module

Fast evaluation of technology investments.

```
class tyche.Evaluator.Evaluator(tranches, summary)
```

Bases: object

Evalutate technology investments using a response surface.

amounts

Cost of tranches.

Type DataFrame

categories

Categories of investment.

Type DataFrame

metrics

Metrics for technologies.

Type DataFrame

units

Units of measure for metrics.

Type DataFrame

interpolators

Interpolation functions for technology metrics.

Type DataFrame

evaluate (amounts)

Sample the distribution for an investment.

Parameters amounts (DataFrame) - The investment levels.

evaluate_statistic (amounts, statistic=<function mean>)

Evaluate a statistic for an investment.

Parameters

- amounts (DataFrame) The investment levels.
- **statistics** (DataFrame) The statistic to evaluate.

12.1.7 tyche.IO module

```
I/O utilities for Tyche.
```

```
tyche.IO.make_table (dtypes, index)
```

Make a data frame from column types and an index.

Parameters

- **dtypes** (array) The column types.
- index (array) The index.

tyche.IO.read_table(path, name, dtypes, index)

Read a data table from a file.

Parameters

- path (str) The path to the folder.
- name (str) The filename for the table.
- **dtypes** (array) The column types.
- index (array) The index.

12.1.8 tyche.Investments module

Investments in technologies.

```
class tyche.Investments.Investments(path=None, tranches='tranches.tsv', invest-
ments='investments.tsv')
```

Bases: object

Investments in a technology.

tranches

The tranches table.

Type DataFrame

investments

The investments table.

Type DataFrame

evaluate_investments (designs, sample_count=1)

Evaluate the investments for a design.

Parameters

- designs (tyche.Designs) The designs.
- **sample_count** (*int*) The number of random samples.

evaluate_tranches (designs, sample_count=1)

Evaluate the tranches of investment for a design.

Parameters

- **designs** (tyche.Designs) The designs.
- **sample_count** (*int*) The number of random samples.

12.1.9 tyche. Types module

```
Data types for Tyche.
```

class tyche.Types.Evaluations (amounts, metrics, summary)

Bases: tuple

Named tuple type for rows in the *evaluations* table.

property amounts

Alias for field number 0

property metrics

Alias for field number 1

property summary

Alias for field number 2

class tyche.Types.FakeDistribution(rvs)

Bases: tuple

Named tuple type for a fake distribution.

property rvs

Alias for field number 0

class tyche.Types.Functions (style, capital, fixed, production, metric)

Bases: tuple

Name tuple type for rows in the *functions* table.

property capital

Alias for field number 1

property fixed

Alias for field number 2

property metric

Alias for field number 4

property production

Alias for field number 3

property style

Alias for field number 0

class tyche.Types.Indices(capital, fixed, input, output, metric)

Bases: tuple

Name tuple type for rows in the *indices* table.

property capital

Alias for field number 0

property fixed

Alias for field number 1

property input

Alias for field number 2

property metric

Alias for field number 4

property output

Alias for field number 3

Bases: tuple

Named tuple type for rows in the *inputs* table.

property input

Alias for field number 2

property input_efficiency

Alias for field number 3

property input_price

Alias for field number 4

property lifetime

Alias for field number 0

property output_efficiency

Alias for field number 5

property output_price

Alias for field number 6

property scale

Alias for field number 1

class tyche.Types.Results(cost, output, metric)

Bases: tuple

Named tuple type for rows in the *results* table.

property cost

Alias for field number 0

property metric

Alias for field number 2

property output

Alias for field number 1

12.1.10 Module contents

Tyche: a Python package for R&D pathways analysis and evaluation.

CHAPTER

THIRTEEN

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