# Tyche Release 1.2

**National Renewable Energy Laboratory** 

# **CONTENTS:**

1	Quick Start Guide	3
2	Technology Model Example	15
3	Analysis Example	21
4	Approach	37
5	Mathematical Formulation	39
6	Optimization	43
7	Python API	51
Pv	thon Module Index	75

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 inform decision-making across R&D projects and programs by assisting analysts and decision makers to 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).

Quick Start Guide covers how to set up an R&D decision context using Tyche by creating the necessary input datasets and writing the technology model. *Technology Model Example* provides a simple example of developing a technology model, and *Analysis Example* provides an analysis example of decision support analysis. High-level information on the approach behind Tyche is given in *Approach* and details on the mathematical formulation used to represent technologies and analyze investment impact is given in *Mathematical Formulation*. *Optimization* gives information on built-in optimization algorithms. The complete Python API for the Tyche codebase and the technology models provided with Tyche is in *Python API*.

CONTENTS: 1

2 CONTENTS:

## **QUICK START GUIDE**

The purpose of this guide is to allow a new user to set up their first R&D decision context using Tyche. An R&D decision context involves one or more technologies that are subject to various R&D investments with the goal of changing the technology metrics and outcomes.

## 1.1 Introduction

The following materials walk through:

- 1. What the Technology Characterization and Evaluation (Tyche) tool does and why this is of value to the user;
- 2. How to set up the Tyche software for local use, including downloading and installing Anaconda;
- 3. How to develop input datasets for a decision context;
- 4. How to develop technology models for a decision context.

# 1.1.1 What does Tyche do?

The Tyche tool provides a consistent and systematic methodology for evaluating alternative R&D investments in a technology or technology system and for comparing the impacts of these investments on metrics and outcomes of interest. Tyche is intended to provide analytical support for funding decision-makers as they consider how to meet their overall goals with various R&D investment strategies.

Tyche's methodology for evaluating and comparing R&D investments:

- 1. Uses techno-economic models of the technology(ies) of interest;
- 2. Incorporates expert elicitation to get quantitative, probabilistic estimates of how the technology(ies) of interest might change with R&D;
- 3. Provides both ensemble simulation and multi-objective stochastic optimization capabilities that enable users to identify R&D investments with the greatest potential for accomplishing decision-maker goals, determine the potential overall improvement in the technology, determine the most promising avenue of R&D for a technology, and more.

For additional details on the mathematics and approach behind Tyche, see the *Mathematical Formulation* and *Approach* sections.

## 1.1.2 What is a "technology"?

In the R&D decision contexts represented and analyzed by Tyche, "technology" has a very broad definition. A technology converts input(s) to output(s) using capital equipment with a defined lifetime, and incurs fixed and/or variable costs in doing so. A technology may be a manufacturing process, a biorefinery, an agricultural process, a renewable energy technology component such as a silicon wafer or an inverter, a renewable energy technology unit such as a wind turbine or solar panel, a renewable power plant system such as a concentrated solar power plant, and more. Within the R&D decision context, a technology is also subject to one or more research areas in which R&D investments can be made to change the technology and its economic, environmental, and other metrics of interest. Multiple technologies can be modeled and compared within the same decision context, provided the same metrics are calculable for each technology. Within Tyche, a technology is represented both physically and economically using a simple but generalized techno-economic analysis (TEA) model. The TEA is based on a user defined technology model and accompanying datasets of technological and investment information.

# 1.2 Getting Started

This section provides guidance on setting up Tyche for use on your local machine. Tyche is written in Python and requires a local Python installation to run. It is recommended to use Anaconda and conda for installing Python and managing Tyche's prerequisite packages.

#### 1.2.1 Install Anaconda

- Download the Anaconda distribution for your system (Windows or MacOS) from the Anaconda Distributions website.
- Once downloaded, follow the instructions provided with the installer.

## 1.2.2 Download the Tyche software

- The latest stable release of the Tyche software can be downloaded as a .zip file from the GitHub repository.
- Extract the files to a location convenient to you. It may be easiest to access these files if they are located on your desktop, but this is not a requirement.

# 1.2.3 Navigate the Tyche directory structure

Once downloaded and extracted, the Tyche files will have the directory structure shown in Fig. 1.1.

- conda contains the environment specification file used to set up the Tyche environment.
- *docs* contains reStructured Text (.rst) files used to generate the Tyche documentation. These files are for internal use only and should not be modified.
- src and its subdirectories contain the Tyche analysis codebase.
  - *technology* contains a subdirectory containing the input datasets (.xlsx) and analysis Jupyter notebooks (.ipynb) for each decision context, as well as the technology model files (.py) for each decision context.
  - *tyche* contains the Python files which provide all of Tyche's functionalities. These files are for internal use only and should not be modified.

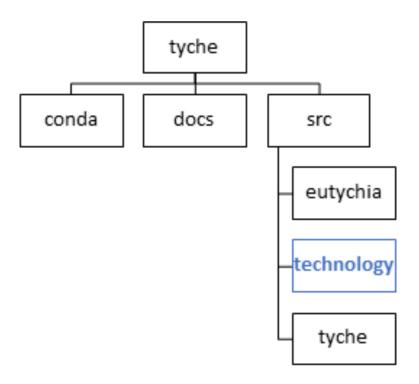


Fig. 1.1: Tyche repository directory structure. New technology models and data should be saved in sub-directories under the technology directory, indicated in blue.

Users creating decision contexts should store the new input datasets, analysis Jupyter notebooks, and technology model files in the technology directory, which is indicated in blue in Fig. 1.1. It is strongly recommended that users create sub-directories for each new decision context, to avoid confusing input datasets and models between contexts.

## 1.2.4 Set up the Tyche environment using conda

Tyche's codebase comes with an environment specification file that is used with Conda to automatically install all of Tyche's required Python packages. It is strongly recommended that users create and use the Tyche environment, to avoid any package conflicts or compatibility issues. It is also recommended that users turn off any VPN before following the steps in this section.

- On Windows, open an Anaconda Prompt (recommended) or Command Prompt window; on Mac, open a System Terminal window.
- Change the current working directory to the location of the extracted Tyche files using cd path/to/tyche/directory.
- Then enter the following commands, pressing Enter after each line:

```
conda env create --file conda\tyche.yml conda activate tyche
```

Note that the first command may take up to 10 minutes to execute. If the environment creation was successful, you should see a message similar to the following:

```
done
#
# To activate this environment, use
(continues on next page)
```

1.2. Getting Started 5

(continued from previous page)

```
#
# $ conda activate tyche
#
# To deactivate an active environment, use
#
# $ conda deactivate
Retrieving notices: ...working... done
```

- If you receive an HTTPS error during environment creation, consider retrying the command with the -insecure flag added.
- See the conda documentation for additional information on installing and troubleshooting environments.

# 1.2.5 Access Tyche analysis functions

Using Tyche locally is generally done via Jupyter Notebook, several examples of which are packaged with the Tyche codebase. To open one of these provided notebooks or to create your own:

- · Open an Anaconda Prompt window.
- Activate the Tyche environment with conda activate tyche.
- Change the current working directory to the location of the extracted Tyche files using cd path/to/tyche/directory.
- Open the Jupyter Notebook browser interface with jupyter notebook.

A browser window or new tab (if a window was already open) will then open and show the files within the Tyche directory, from which existing notebooks can be opened and run or new notebooks created.

# 1.3 Defining a Decision Context

After Tyche and its prerequisites are installed, the user can begin assembling the input datasets and technology models necessary for running their own decision context analyses. This section provides details on the contents of each input dataset required by Tyche and on the structure and function of the technology model (.py) file.

Tyche contains built-in data validation checks that, once run, will provide a list of any data inconsistencies or apparent errors as well as the names of the datasets in which the inconsistencies were found. Users are encouraged to review the information here to create a first draft of their input datasets, and then rely on the validation checks for additional troubleshooting. Users may also find it helpful to begin developing their input datasets by altering and adding to one of the decision context datasets packaged with Tyche, rather than starting from scratch.

An example technology model is developed in the *Technology Model Example* section, and an example of using Tyche for decision support analysis is provided in the *Analysis Example* section.

## 1.3.1 Technology Data and Model

## **Designs Dataset**

A "design" is a set of data representing the state of a technology that results from a specific R&D investment scenario. The *designs* dataset contains information for all of the technologies being evaluated within a decision context. *designs* contains multiple sets of data for each technology: each set represents the technology state that results from a single R&D investment scenario. Multiple R&D investment scenarios are typically represented, each corresponding to a different level of technology advancement, which is quantified probabilistically through expert elicitation. Table 1.1 provides a data dictionary for the *designs* dataset.

Table 1.1: Data dictionary for the *designs* dataset which defines various technology states resulting from R&D investments.

Column Name	Data Type	Allowed Values	Description
Technology	String	Any	Name of the technology.
Scenario	String	Any names are allowed. There must be at least two scenarios defined.	R&D investment scenario that results in this technology design.
Variable	String	<ul> <li>Input</li> <li>Input efficiency</li> <li>Input price</li> <li>Output efficiency</li> <li>Output price</li> <li>Lifetime</li> <li>Scale</li> </ul>	Variable types required by technology model and related functions.
Index	String	Any	Name of the elements within each Variable.
Value	<ul><li> Float</li><li> Distribution</li><li> Mixture of distributions</li></ul>	Set of real numbers     scipy.stats distributions     Mixture of scipy.stats distributions	Value for the R&D investment scenario. Example: st.triang(1,loc=5,scale=0.1)
Units	String	Any	User defined units for Variables. Not used by Tyche.
Notes	String	Any	Description provided by user. Not used by Tyche.

**Mandatory data.** The Variable column within the *designs* dataset must contain all seven values defined in Table 1.1. If there are no elements within a Variable for the technology under study, the Variable must still be included in the *designs* dataset: leaving out any of the Variables in this dataset will result in the *designs* dataset failing the data validation checks. The Value for unneeded Variables may be set to 0 or 1, and the Index for unneeded Variables set to None. This may be necessary for technologies without any inputs: for instance, a solar panel could be modeled without any Inputs, if sunlight is not explicitly being modeled. In this case, the single Index defined for the Input Variable can be None, and the calculations within the technology model .py file can be defined without using this value. The mandatory Variables and their component Indexes are defined further in Table 1.2.

	Table 1.2. Mandatory values it	or variables in the designs dataset.
Vari-	Description	Index Description
able		
Input	Ideal input amounts that do not account for	Names of inputs to the technology.
	inefficiencies or losses.	
Input	Input inefficiencies or losses, expressed as a	Names of inputs to the technology: every input with an
effi-	number between 0 and 1.	amount must also have an efficiency value, even if the ef-
ciency		ficiency is 1.
Input	Purchase price for the input(s)	Names of inputs to the technology.
price		
Output	Output efficiencies or losses, expressed as a	Names of outputs from the technology. Every output must
effi-	number between 0 and 1.	have an efficiency value, even if the efficiency is 1.
ciency		
Output	Sale price for the output(s).	Names of outputs from the technology. Every output must
price		have a price, even if the price is irrelevant (in which case,
		set the price to 0).
Life-	Time that a piece of capital spends in use;	Names of the capital components of the technology.
time	time it takes for a piece of capital's value to	
	depreciate to zero.	
Scale	Scale at which the technology operates (one	No index.
1		<u> </u>

Table 1.2: Mandatory values for Variables in the designs dataset.

#### **Parameters Dataset**

value for the technology).

The *parameters* dataset contains any additional technology-related data, other than that contained in the *designs* dataset, that is required to calculate a technology's capital cost, fixed cost, production (actual output amounts), and metrics. (These calculations are implemented within the technology model .py file, discussed in the next section.) Identically to the *designs* dataset, the *parameters* dataset contains multiple sets of data corresponding to different R&D investment scenarios. A data dictionary for the *parameters* dataset is given in Table 1.3.

Table 1.3: Data dictionary for the *parameters* dataset, which, if necessary, provides additional technology-related data other than that in the *designs* dataset.

Column	Data type	Description					
Name							
Technol-	String	Name of the technology.					
ogy							
Scenario	String	Name of the R&D investment scenario that resulted in the correspond-					
		ing parameter values or distributions.					
Parameter	String	Name of the parameter.					
Offset	Integer	Numerical location of the parameter in the parameter vector; begins at					
		zero.					
Value	Float; Distribution; Mixture	Parameter value for the R&D investment scenario. Example:					
	of distributions	st.triang(1,loc=5,scale=0.1)					
Units	String	Parameter units. User defined; not used or checked during Tyche cal-					
		culations.					
Notes	String	Any additional information defined by the user. Not used during Tyche					
		calculations.					

Including the Offset value in the *parameters* dataset creates a user reference that makes it easier to access parameter values when defining the technology model.

**Mandatory data.** The *parameters* dataset is required to exist and to include at least one Parameter for every Technology-Scenario combination. If there are no Parameters present in the technology model, then the Parameter may be None and 0 may be entered under both the Offset and Value columns.

## Technology model (.py file)

The technology model is a Python file (.py) which is user defined and contains methods for calculating capital cost, fixed cost, production (the actual output amount), and any metrics of interest, using the content of the *designs* and *parameters* datasets. Table 1.4 describes methods that must be included in the technology model. Additional methods can be included in the technology model, if necessary. The names of the mandatory methods in Table 1.4 are user-defined and must match the contents of the *functions* dataset, discussed below. The method parameters listed in Table 1.4 are also fixed and cannot be changed. In the case that a method does not require all of the mandatory input parameters, they can simply be left out of the method's calculations.

Table 1.4: Methods required within the technology model Python file. Method names are user-defined and should match the contents of the functions dataset. Additional methods can be defined within the technology model as necessary.

Recommended Method Name	Parameters (method inputs)	Returns
capital_cost	scale, parameter	Capital cost(s) for each type of
		capital in the technology.
fixed_cost	scale, parameter	Annual fixed cost(s) of operating
		the technology.
production	scale, capital, lifetime, fixed, input, parameter	Calculated actual (not ideal) out-
		put amount(s).
metrics	scale, capital, lifetime, fixed, input_raw, input, in-	Calculated technology metric
	put_price, output_raw, output, cost, parameter	value(s).

The production method can access the actual input amount, which is the ideal or raw input amount value multiplied by the input efficiency value (both defined in the *designs* dataset). In contrast, the metrics method can access both the ideal input amount (input\_raw) and the actual input amount (input).

All return values for the required methods, even if only a single value is returned, must be formatted as Numpy stacks.

Part of Tyche's analysis capabilities rely on the ability to evaluate the impact of multiple R&D investments across research areas. In order for the R&D investment impacts to be combined, it is recommended that the return values for the metrics method be represented as changes from a baseline value that represents the current state of technology. These changes can then be summed across R&D investments to see the overall impact.

## 1.3.2 Investment Datasets

The previous sections provided information on the input datasets required to define the technology(ies) of interest within a decision context, and on the content and structure of the technology model itself. This section provides information on the input datasets that define R&D investment options and the research categories in which investments can be made.

#### **Tranches Dataset**

A Tranche is a discrete unit of R&D investment (dollar amount) in a specific research category. Research categories are defined for each technology within a decision context and represent narrow topic areas in which R&D investments are expected to result in technological improvements. Tranches within the same research category are mutually exclusive: one cannot simultaneously invest \$1M and \$5M in a research category. A Scenario is a combination of Tranches that represents one option for making R&D investments.

The *tranches* dataset defines a set of R&D investments across the research categories that are relevant to the technology under study. Tranches are combined into investment Scenarios – the same Scenarios found in the *designs* and *parameters* datasets. The impact of each Scenario on the technology is highly uncertain and is quantified probabilistically using expert elicitation. A data dictionary for the *tranches* dataset is given in Table 1.5.

Col-	Data Type	Description
umn		
Name		
Cate-	String	Names of the R&D categories in which investment can be made to impact the tech-
gory		nology or technologies being studied.
Tranche	String	Names of the tranches.
Sce-	String	Names of the R&D investment scenarios, which combine tranches across R&D cat-
nario		egories. The names in this column must correspond to the Scenarios listed in the
		designs and parameters datasets.
Amount	Float; Distribu-	The R&D investment amount of the Tranche. The amount may be defined as a scalar,
	tion; Mixture of	a probability distribution, or a mix of probability distributions.
	distributions	
Notes	String	Additional user-defined information. Not used by Tyche.

Table 1.5: Data dictionary for the *tranches* dataset.

## **Investment Dataset**

An Investment, similar to a Scenario, is a combination of Tranches that represents a particular R&D strategy.

The *investments* dataset provides a separate way to look at making R&D investments. Combining individual tranches allows users to explore and optimize R&D investment amounts, but it may be the case that there are specific strategies that users wish to explore, without optimizing. In this case, the *investments* dataset is used to define specific combinations of tranches that are of interest. A data dictionary for the *investments* dataset is given in Table 1.6.

		,
Col-	Data Type	Description
umn		
Name		
Invest-	String	Name of the R&D investment. Distinct from the Scenarios.
ment		
Cate-	String	Names of the R&D categories being invested in. Within each row, the Category must
gory		match the Tranche. The set of Categories in the <i>investments</i> dataset must match the set of
		Categories in the <i>tranches</i> dataset.
Tranche	String	Names of the tranches within the Investment. Within each row, the Tranche must match
		the Category. The set of Tranches in the <i>investments</i> dataset must match the set of Tranches
		in the <i>tranches</i> dataset.
Notes	String Addition	nal user-defined information. Not used by Tyche.

Table 1.6: Data dictionary for the *investments* dataset.

**Relationship between Categories, Tranches, Scenarios, and Investments.** Both the *designs* and *parameters* dataset contain technology data under multiple Scenarios. Each Scenario represents the technological outcomes from one or more

Tranches, and each Tranche represents a unit of R&D investment in a single Category (or research area). Scenarios and their component Tranches are defined in the *tranches* dataset. Tranches can also be combined to form Investments, as defined in the *investments* dataset.

#### 1.3.3 Additional Datasets

#### **Indices Dataset**

The *indices* dataset contains the numerical indexes (location within a list or array) used to access content in the other datasets. Table 1.7 describes the columns required for the indices table. Numerical locations for parameters should not be listed in this dataset.

Column Name	Data Type	Allowed Values	Description
Technology	String	Any	Name of the technology
Туре	String	<ul><li>Capital</li><li>Input</li><li>Output</li><li>Metric</li></ul>	Names of the Types defined within the designs dataset.
Index	String	Any	Name of the elements within each Type. For instance, names of the Input types.
Offset	Integer	>= 0	Numerical location of the Index within each Type.
Description	String	Any	Additional user-defined information, such as units.  Not used during Tyche calculations.
Notes	String	Any	Additional user-defined information. Not used during Tyche calculations.

Table 1.7: Data dictionary for the indices dataset.

Relationship between \*indices\* and other datasets. A technology in the Tyche context is quantified using five sets of attribute values and one technology-level attribute value. The five sets of attribute values are Capital, Input, Output, Parameter, and Metric, and the technology-level attribute is Scale. Elements within each of the five sets are defined with an Index which simply names the element (for instance, Electricity might be one of the Index values within the Input set). Elements of Capital have an associated Lifetime. Elements of the Input set have an associated ideal amount (also called Input), an Input efficiency value, and an Input price. Elements of the Output set have only an Output efficiency and an Output price; the ideal output amounts are calculated from the technology model. Elements of the Metric set are named with an Index and are likewise calculated from the technology model. Elements of the Parameter set have only a value. The *indices* dataset lists the elements of the Capital, Input, Output, and Metric sets, and contains an Offset column giving the numerical location of each element within its set. The *designs* dataset contains values for each element of the Capital, Input, Output, and Metric sets as well as the technology-level Scale value. The *parameters* dataset names and gives values for each element of the Parameter set.

**Mandatory data.** All four Types must be listed in the *indices* dataset. If a particular Type is not relevant to the technology under study, it still must be included in this dataset.

#### **Functions Dataset**

The *functions* dataset is used internally by Tyche to locate the technology model file and identify the four required methods listed in Table 1.4. Table 1.8 provides a data dictionary for the *functions* dataset.

Column Data Allowed Description Name Type Values Technol-String Any Name of the technology. ogy Style See below for explanation. String numpy Module String Any Filename of the technology model Python file. Do not include the file exten-Capital Name of the method within the technology model Python file that returns the String Any calculated capital cost. Fixed Name of the method within the technology model Python file that returns the String Any calculated fixed cost. Production String Any Name of the method within the technology model Python file that returns the calculated output amount. Name of the method within the technology model Python file that returns the Metrics String Any calculated technology metrics. Notes Any information that the user needs to record can go here. Not used during String Any

Table 1.8: Data dictionary for the *functions* dataset.

The Style should remain *numpy* for all Tyche versions 1.x. This indicates that inputs and outputs from the methods within the technology model Python file are treated as arrays rather than higher-dimensional (i.e., tensor) structures.

If only one technology model is used within a decision context, then the *functions* dataset will contain a single row.

Tyche calculations.

#### **Results Dataset**

The *results* dataset lists the Tyche outcomes that are of interest within a decision context, organized into categories defined by the Variable column. This dataset is used internally by Tyche for organizing and labeling results tables for easier user comprehension. A data dictionary for the *results* dataset is given in Table 1.9.

Column Name	Data Type	Allowed Values	Description
Technology	String	Any	Name of the technology.
Variable	String	<ul><li> Cost</li><li> Output</li><li> Metric</li></ul>	Specific technology outcomes calculated by Tyche.
Index	String	Any	Names of the elements within each Variable.
Units	String	Any	User-defined units of the Index values. Not used or checked during Tyche calculations.
Notes	String	Any	Additional information defined by the user. Not used during Tyche calculations.

Table 1.9: Data dictionary for the results dataset.

The Variable Cost is a technology-wide lifetime cost, and as such may not be relevant within all decision contexts. The Index of Cost can be simply Cost. The sets of Index values for the Output and Metric Variables should match the Output and Metric sets in both the *designs* and the *indices* datasets.

**Mandatory data.** Every Index within the Cost, Output and Metric sets defined elsewhere in the input datasets should be included in the *results* dataset.

# 1.4 Uncertainty in the Input Datasets

Tyche provides two general use cases for exploring the relationship between R&D investments and technological changes, both of which rely on expert elicitation to quantify inherent uncertainty. In the first and likely more common use case, a user knows what the R&D investment options are for a technology or set of technologies and is interested in determining what impact these investment options have on the technology(ies) in order to decide how to allocate an R&D budget. In other words, in this use case the user already knows the contents of the *tranches* and *investments* datasets, which are deterministic (fixed), and uses expert elicitation to fill in key values in the *designs* and *parameters* datasets with probability distributions.

In the second use case, a user knows what technological changes must be achieved with R&D investment and is interested in determining the investment amount that will be required to achieve these changes. In this case the user already knows the contents of the *designs* and *parameters* dataset, which are deterministic, and uses expert elicitation to fill in the investment amounts in the *tranches* dataset.

It is critical to note that these use cases are **mutually exclusive**. Tyche cannot be used to evaluate a scenario in which desired technological changes as well as the investment amounts are both uncertain. What this means for the user is that probability distributions, or mixtures of distributions, can be used to specify values either in the *designs* and *parameters* datasets or in the *tranches* dataset, but not both. If distributions are used in all three datasets, the code will break by design.

# 1.4.1 Defining values as probability distributions and mixtures

An uncertain value can be defined within a dataset using any of the built-in distributions of the scipy.stats package. A list of available distributions is provided at the hyperlink. Uncertain values can also be defined as a weighted average or mixture of probability distributions using the Tyche *mixture* method.

## TECHNOLOGY MODEL 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  $H_2$ :

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

For this example, we treat the catalyst as the capital that we use to transform inputs into outputs. Our inputs are water and electricity, and our outputs are oxygen and hydrogen. Our only fixed cost is the rent on the lab space at \$1000/year. Using our past experience with electrolysis technology as well as some historical data, we estimate that we'll be able to produce 6650 mol/year of hydrogen and at this scale, our catalyst has a lifetime of about 3 years. The metrics we'd like to calculate for our electrolysis technology are cost, greenhouse gas (GHG) emissions, and jobs created. Based on this information, the *designs* dataset for the base case electrolysis technology is as shown in Table 2.1.

Table 2.1: *designs* dataset for the base case (without any R&D) of the simple electrolysis example technology.

Technol	ogy	Scena	rio	Variable		Index	Value	Units	Notes
Simple	elec-	Base	Elec-	Input		Water	19.04	g/mole	
trolysis		trolysis							
Simple	elec-	Base	Elec-	Input	effi-	Water	0.95	1	Due to mass transport loss on
trolysis		trolysis		ciency					input.
Simple	elec-	Base	Elec-	Input		Elec-	279	kJ/mole	
trolysis		trolysis				tricity			
Simple	elec-	Base	Elec-	Input	effi-	Elec-	0.85	1	Due to ohmic losses on input.
trolysis		trolysis		ciency		tricity			
Simple	elec-	Base	Elec-	Output	effi-	Oxygen	0.9	1	Due to mass transport loss on
trolysis		trolysis		ciency					output.
Simple	elec-	Base	Elec-	Output	effi-	Hydro-	0.9	1	Due to mass transport loss on
trolysis		trolysis		ciency		gen			output.
Simple	elec-	Base	Elec-	Lifetime		Catalyst	3	yr	Effective lifetime of Al-Ni
trolysis		trolysis							catalyst.
Simple	elec-	Base	Elec-	Scale		n/a	6650	mole/yr	Rough estimate for a 50W
trolysis		trolysis							setup.
Simple	elec-	Base	Elec-	Input price	ce	Water	4.80E-	USD/mole	;
trolysis		trolysis					03		
Simple	elec-	Base	Elec-	Input price	ce	Elec-	3.33E-	USD/kJ	
trolysis		trolysis				tricity	05		
Simple	elec-	Base	Elec-	Output pi	rice	Oxygen	3.00E-	USD/g	
trolysis		trolysis					03		
Simple	elec-	Base	Elec-	Output pi	rice	Hydro-	1.00E-	USD/g	
trolysis		trolysis				gen	02		

Note that this is not the only way to model the electrolysis technology. We could choose to purchase lab space and

equipment instead of renting, in which case we would have more types of capital, each with a particular lifetime. We could treat the oxygen output from our technology as waste instead of a coproduct and remove it from the model entirely. We could operate at a different scale and perhaps change our fixed or capital costs by doing so. Depending on where we operate this technology, our input and output prices will likely change. The Tyche framework offers great flexibility in representing technologies and technology systems; it is unlikely that there will only be a single correct way to model a decision context.

A key quantity that is not included in the *designs* dataset is our fixed cost, rent for the lab space. This quantity is included in the *parameters* dataset in Table 2.2, along with the necessary data to calculate our metrics of interest (cost, GHG, jobs).

Table 2.2: *parameters* dataset for the base case (without any R&D) of the simple electrolysis example technology.

Technology	Scenario	Parameter	Off-	Value	Units	Notes
			set			
Simple elec-	Base Elec-	Oxygen production	0	16	g	
trolysis	trolysis					
Simple elec-	Base Elec-	Hydrogen production	1	2	g	
trolysis	trolysis					
Simple elec-	Base Elec-	Water consumption	2	18.08	g	
trolysis	trolysis					
Simple elec-	Base Elec-	Electricity consumption	3	237	kJ	
trolysis	trolysis					
Simple elec-	Base Elec-	Jobs	4	1.50E-	job/mole	
trolysis	trolysis			04		
Simple elec-	Base Elec-	Reference scale	5	6650	mole/yr	
trolysis	trolysis					
Simple elec-	Base Elec-	Reference capital cost	6	0.63	USD	
trolysis	trolysis	for catalyst				
Simple elec-	Base Elec-	Reference fixed cost for	7	1000	USD/yr	
trolysis	trolysis	rent				
Simple elec-	Base Elec-	GHG factor for water	8	0.00108	gCO2e/g	
trolysis	trolysis					Mg CO2e
Simple elec-	Base Elec-	GHG factor for electric-	9	0.138	gCO2e/k	Jbased on 1 kWh = $0.5 \text{ kg}$
trolysis	trolysis	ity				CO2e

Within our R&D decision context, we're interested in increasing the input and output efficiencies of this process so we can produce hydrogen as cheaply as possible. Experts could assess how much R&D to increase the various efficiencies  $\eta$  would cost. They could also suggest different catalysts, adding alkali, or replacing the process with PEM.

The indices table (see Table 2.3) 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.

Table 2.3: Example of the indices table.

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	

# 2.1 Production function (à la Leontief)

$$\begin{split} P_{\text{oxygen}} &= (16.00 \text{ g}) \cdot \min \left\{ \frac{I_{\text{water}}^*}{18.08 \text{ g}}, \frac{I_{\text{electricity}}^*}{237 \text{ kJ}} \right\} \\ P_{\text{hydrogen}} &= (2.00 \text{ g}) \cdot \min \left\{ \frac{I_{\text{water}}^*}{18.08 \text{ g}}, \frac{I_{\text{electricity}}^*}{237 \text{ kJ}} \right\} \end{split}$$

## 2.2 Metric functions

```
\begin{split} M_{\rm cost} &= K/O_{\rm hydrogen} \\ M_{\rm GHG} &= \left( (0.00108~{\rm gCO2e/gH20})~I_{\rm water} + (0.138~{\rm gCO2e/kJ})~I_{\rm electricity} \right)/O_{\rm hydrogen} \\ M_{\rm iobs} &= \left( 0.00015~{\rm job/mole} \right)/O_{\rm hydrogen} \end{split}
```

# 2.3 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_{\rm hydrogen}=1.8~{\rm g/mole} \mu_{\rm cost}=0.102~{\rm USD/gH2} \mu_{\rm GHG}=21.4~{\rm gCO2e/gH2} \mu_{\rm jobs}=0.000083~{\rm job/gH2}
```

# 2.4 Technology Model

Each technology design requires a Python file with a capital cost, a fixed cost, a production, and a metrics function. Listing 2.1 shows these functions for the simple electrolysis example.

Listing 2.1: 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])
    )])
```

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```
# 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
):
  # Moles of input.
          = 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.
```

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```
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])
```

**CHAPTER** 

**THREE** 

## **ANALYSIS EXAMPLE**

Multiple Objectives for Residential PV.

# 3.1 Import packages.

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

```
import numpy    as np
import matplotlib.pyplot as pl
import pandas    as pd
import seaborn    as sb
import tyche    as ty

from copy    import deepcopy
from IPython.display import Image
```

## 3.2 Load data.

The data should be stored in a set of comma-separated value files in a sub-directory of the technology folder, as shown in the directory structure diagram (Fig. 1.1)

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

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

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

```
designs.compile()
```

# 3.3 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

# 3.4 Evaluate the scenarios in the dataset.

scenario\_results = designs.evaluate\_scenarios(sample\_count=50)

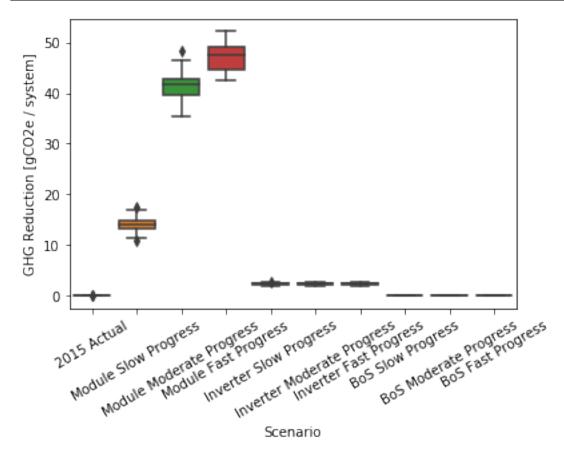
scenario\_results.xs(1, level="Sample", drop\_level=False)

## 3.4.1 Save results.

scenario\_results.to\_csv("output/pv\_residential\_simple/example-scenario.csv")

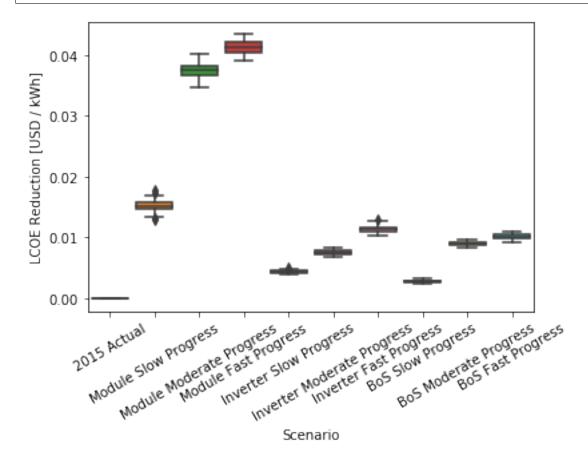
## 3.4.2 Plot GHG metric.

```
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);
```



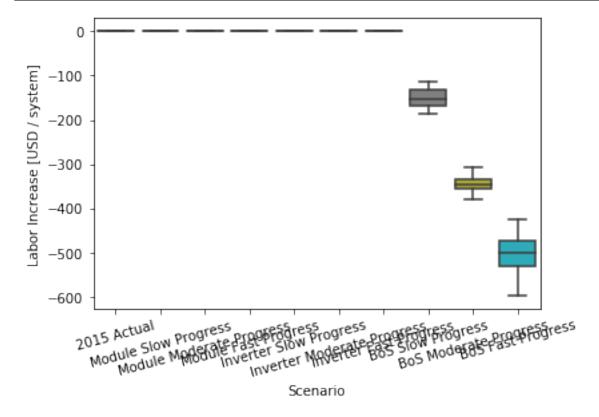
## 3.4.3 Plot LCOE metric.

```
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);
```



## 3.4.4 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);
```



# 3.5 Evaluate the investments in the dataset.

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

#### 3.5.1 Costs of investments.

```
investment_results.amounts
```

#### 3.5.2 Benefits of investments.

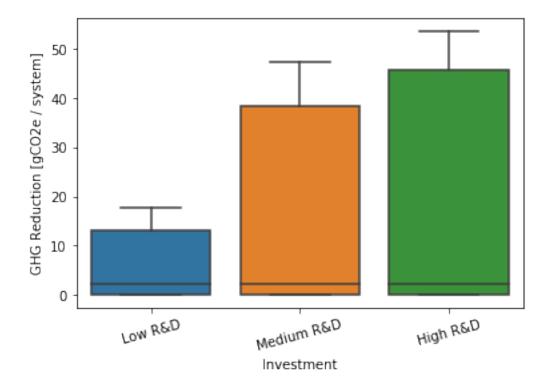
```
investment_results.metrics.xs(1, level="Sample", drop_level=False)
```

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

## 3.5.3 Save results.

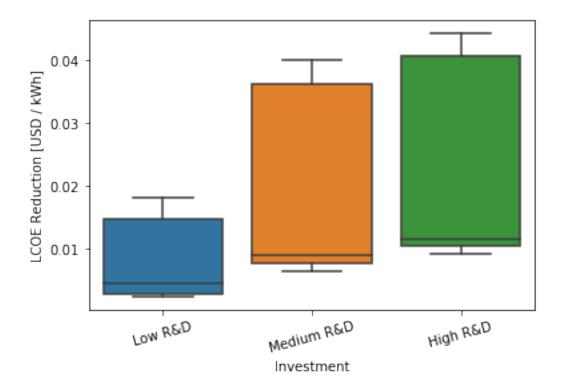
# 3.5.4 Plot GHG metric.

```
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);
```



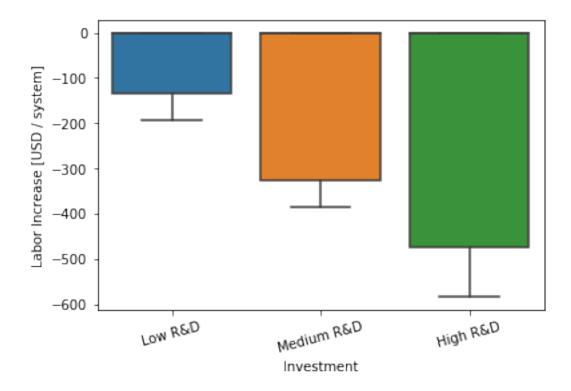
## 3.5.5 Plot LCOE metric.

```
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);
```



## 3.5.6 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);
```



# 3.6 Multi-objective decision analysis.

# 3.6.1 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.

## 3.6.2 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
```

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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
```

## 3.6.3 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  $\varepsilon$ -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
```

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

```
optimum.metrics
```

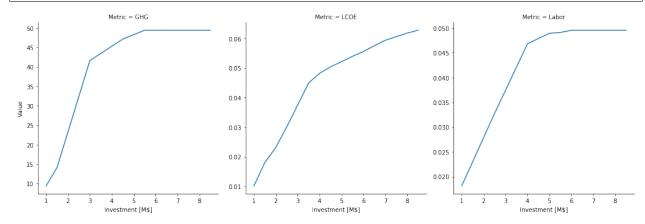
```
Index
GHG 39.046988
LCOE 0.036463
Labor -0.019725
Name: Value, dtype: float64
```

## 3.6.4 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>
```

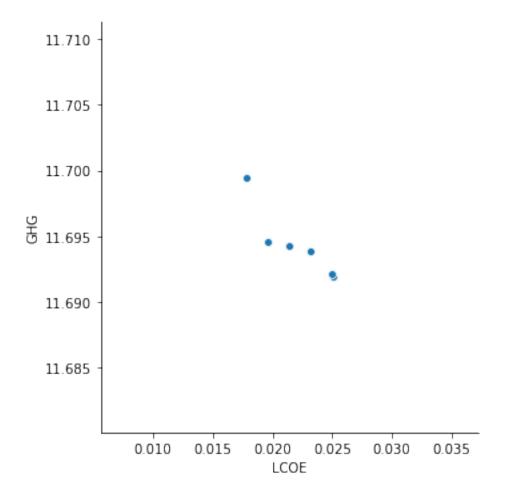


We see that the LCOE metric saturates more slowly than the GHG and Labor ones.

## 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
```

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



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.

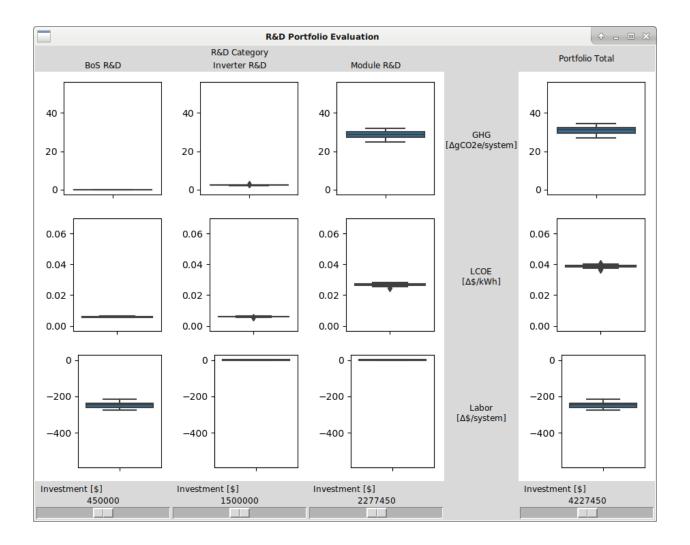
# 3.7 Run the interactive explorer for the decision space.

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("pv_residential_simple_gui.png")
```



**CHAPTER** 

# **FOUR**

## **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 laptop computers 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 simulation or subsequent to it.

Four example technologies have been implemented as examples illustrating the 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 5.1 defines the indices that are used for the variables that are defined in Table 5.2.

Table 5.1: 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 5.2: 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
$\eta_i$	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
$\eta_o'$	waste	output efficiency	output/output
$p'_o$	cost	output price (+/-)	USD/output
$\mu_m$	calculated	metric	metric/unit
$P_o$	function	production function	output/unit

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Variable	Туре	Description	Units
$M_m$	function	metric function	metric/unit
$\alpha_p$	parameter	technical parameter	(mixed)
$\xi_{\theta}$	variable	scenario inputs	(mixed)
$\zeta_{\theta}$	variable	scenario outputs	(mixed)
$\psi$	function	scenario evaluation	(mixed)
$\sigma_{\phi}$	function	scenario probability	1
$q_{\phi}$	variable	investment cost	USD
$\zeta_{\phi}$	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
$q_{\phi}^{\max}$	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 5.2 - continued from previous page

# **5.1 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:

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

# 5.2 Waste

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

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

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

# 5.3 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.

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

## 5.4 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.

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

## 5.5 Scenarios

A scenario represents a state of affairs for a technology  $\nu$ . If we denote the scenario as  $\theta$ , 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.

## 5.6 Investments

An *investment*  $\phi$  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  $\zeta_{\phi}$  as a random variable for the outcomes  $\zeta_{\theta}$  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  $\Phi_{\chi}$  is the set of mutually exclusive investments (i.e., only one can occur simultaneously) in investment category  $\chi$ : investments in different categories  $\chi$  can be combined arbitrarily, but just one investment from each  $\Phi_{\chi}$  may be chosen.

5.3. Production 41

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  $\phi$  is  $q_{\phi}$ , so the cost of a portfolio is:

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

# 5.7 Decision problem

The multi-objective decision problem is

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

such that

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

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

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

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

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

# 5.8 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  $\theta$  of each investment  $\phi$ .

## **OPTIMIZATION**

# **6.1 Nonlinear Programming Formulation**

Three methods in the EpsilonConstraintOptimizer class, opt\_slsqp, opt\_shgo and opt\_diffev, are wrappers for optimization algorithm calls. (The *tyche.EpsilonConstraints* section provides full parameter and return value information for these methods.) 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. Because the technology models within an R&D decision context may be arbitrarily complex, two global optimization algorithms were also implemented. The global algorithms were chosen according to the following criteria.

- Ability to perform constrained optimization with inequality constraints, for instance on metric values or investment amounts.
- Ability to optimize without specified Jacobian or Hessian functions (derivative-less optimization).
- · Ability to specify bounds on individual decision variables, which allows constraints on single research areas.
- Ability to work on a variety of potentially non-convex and otherwise complex problems.

## 6.1.1 Algorithm Testing

As a point of comparison between algorithms, the *Simple Residential Photovoltaics* decision context was optimized for minimum levelized cost of electricity (LCOE) subject to an investment constraint and a metric constraint (GHG). The solutions are given in Table 6.1. The solve times listed are in addition to the time required to set up the problem and solve for the optimum metric values; this procedure currently uses the SLSQP algorithm by default. This setup time is between 10 and 15 seconds.

Table 6.1: Minimizing LCOE subject to a total investment amount of \$3 MM USD and GHG being at least 40.

Algorithm	Objective Function Value	GHG Constraint Value	Solve Time (s)
Differential evolution	0.037567	41.699885	145
Differential evolution	0.037547	41.632867	589
SLSQP	0.037712	41.969348	~ 2
SHGO	None found	None found	None found

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

# 6.2 Sequential Least Squares Programming (SLSQP)

The Sequential Least Squares Programming algorithm uses a gradient search method to locate a possibly local optimum. [6] A complete list of parameters and options for the fmin\_slsqp algorithm is available in the scipy.optimize.fmin\_slsqp documentation.

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.

# 6.2.1 SLSQP Solution to Simple Residential Photovoltaics

Solve time: 1.5 s

Table 6.2: Optimal decision variables found by the SLSQP algorithm.

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

Table 6.3: Optimal system metrics found by the SLSQP algorithm.

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. Moreover, users may need to adjust the default solving parameters and options in order to obtain a solution and cut down on solve time. A complete list of parameters and options for the *differential\_evolution* algorithm is available in the scipy.optimize.differential\_evolution documentation.

Constraints for differential\_evolution are defined by passing the same multi-valued function defined in opt\_slsqp to the NonlinearConstraint method.

## 6.3.1 Differential Evolution Solutions to Simple Residential Photovoltaics

Differential evolution stochastically populates the initial set of potential solutions, and so the optimal solution and solve time may vary with the random seed used.

### Solution 1

Starting with a random seed of 2, the solution time was 145 seconds.

Table 6.4: Optimal decision variables found by the differential evolution algorithm with a seed of 2.

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

Table 6.5: Optimal system metrics found by the differential evolution algorithm with a seed of 2.

System Metric	Optimized Value
GHG	41.70
LCOE	0.038
Labor	-0.456

#### Solution 2

Starting with a random seed of 1, the solution time was 589 seconds.

Table 6.6: Optimal decision variables found by *differential\_evolution* as called by *EpsilonConstraints.opt\_diffev* with a seed of 1.

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

Table 6.7: Optimal system metrics found by *differential\_evolution* as called by *EpsilonConstraints.opt\_diffev* with a seed of 1.

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] SHGO provides fast solutions using default parameters and options, but the optimum found may not be as precise as that found by the differential evolution algorithm. Constraints for *shgo* must be provided as a dictionary or sequence of dictionaries with the following format:

(continues on next page)

(continued from previous page)

```
{'type': 'eq', 'fun': h2(x)},
... ]
```

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

# 6.5 Piecewise Linear (MILP) Formulation

## 6.5.1 Notation

Table 6.8: Index definitions for the MILP formulation.

Index	Description
I	Number of elicited data points (investment levels and metrics)
J	Number of investment categories
K	Number of metrics

Table 6.9: Data definitions for the MILP formulation.

Data	Notation	Information
Investment	$c_{ij}, i \in \{1,, I\}$	$c_i$ is a point in $J$ -dimensional space
amounts		
Metric value	$q_{ik}, i \in \{1,, I\}, k \in$	One metric will form the objective function, leaving up to $K-1$
	$\mid \{1,,K\}$	metrics for constraints

Table 6.10: Variable definitions for the MILP formulation.

Variable	Notation	Information
Binary variables	$y_{ii'}, i, i' \in$	Number of linear intervals between elicited data points.
	$\{1,, I\}, i' > i$	
Combination vari-	$\lambda_i, i \in \{1,, I\}$	Used to construct linear combinations of elicited data points.
ables		$\lambda_i \ge 0 \forall i$

Each metric and investment amount can be written as a linear combination of elicited data points and the newly introduced variables  $\lambda_i$  and  $y_{ii'}$ . Additional constraints on  $y_{ii'}$  and  $\lambda_i$  take care of the piecewise linearity by ensuring that the corners used to calculate  $q_k$  reflect the interval that  $c_i$  is in. There will be a total of  $\binom{I}{2}$  binary y variables, which reduces to  $\frac{I(I-1)}{2}$  binary variables.

## 6.5.2 One-Investment-Category, One-Metric Example

Suppose we have an elicited data set for one metric (K = 1) and one investment category (J = 1) with three possible investment levels (I = 3). We can write the total investment amount as a linear combination of the three investment levels  $c_{i1}$ ,  $i \in \{1, 2, 3\}$ , using the  $\lambda$  variables:

$$\lambda_1 c_{11} + \lambda_2 c_{21} + \lambda_{13} c_{31} = \sum_i \lambda_i c_{i1}$$

We can likewise write the metric as a linear combination of  $q_{1i}$  and the  $\lambda$  variables:

$$\lambda_1 q_{11} + \lambda_2 q_{21} + \lambda_3 q_{31} = \sum_i \lambda_i q_{i1}$$

We have the additional constraint on the  $\lambda$  variables that

$$\sum_{i} \lambda_i = 1$$

These equations, combined with the integer variables  $y_{ii'} = \{y_{12}, y_{13}, y_{23}\}$ , can be used to construct a mixed-integer linear optimization problem.

The MILP that uses this formulation to minimize a technology metric subject to a investment budget B is as follows:

$$\min_{y,\lambda} \lambda_1 q_{11} + \lambda_2 q_{21} + \lambda_3 q_{31}$$

subject to

 $\lambda_1 c_{11} + \lambda_2 c_{21} + \lambda_3 c_{31} \leq B$ , (1) Total budget constraint

$$\lambda_1 + \lambda_2 + \lambda_3 = 1, (2)$$

$$y_{12} + y_{23} + y_{13} = 1$$
, (3)

$$y_{12} \leq \lambda_1 + \lambda_2$$
, (4)

$$y_{23} \leq \lambda_2 + \lambda_3$$
, (5)

$$y_{13} \leq \lambda_1 + \lambda_3$$
, (6)

$$0 \leq \lambda_1, \lambda_2, \lambda_3 \leq 1$$
, (7)

$$y_{12}, y_{23}, y_{13} \in \{0, 1\}$$
, (8)

(We've effectively removed the investments and the metrics as variables, replacing them with the elicited data points and the new  $\lambda$  and y variables.)

### 6.5.3 Extension to N x N Problem

Note: k' indicates the metric which is being constrained. k\* indicates the metric being optimized. J' indicates the set of investment categories which have a budget limit (there may be more than one budget-constrained category in a problem).

No metric constraint or investment category-specific budget constraint

$$\min_{y,\lambda} \sum_{i} \lambda_{i} q_{ik*}$$

subject to

$$\sum_{i} \sum_{j} \lambda_{i} c_{ij} \leq B$$
, (1) Total budget constraint

$$\sum_{i} \lambda_i = 1$$
, (2)

$$\sum_{i,i'} y_{ii'} = 1$$
, (3)

$$y_{ii'} \leq \lambda_i + \lambda_{i'} \forall i, i', (4)$$

$$0 \le \lambda_i \le 1 \forall i$$
, (5)

$$y_{ii'} \in \{0,1\} \forall i,i',(6)$$

## With investment category-specific budget constraint

$$\min_{y,\lambda} \sum_{i} \lambda_{i} q_{ik*}$$

subject to

 $\sum_{i} \sum_{j} \lambda_{i} c_{ij} \leq B$ , (1) Total budget constraint

 $\sum_{i} \lambda_{i} c_{ij'} \leq B_{j'} \forall j' \in J'$ , (2) Investment category budget constraint(s)

$$\sum_{i} \lambda_{i} = 1$$
, (3)

$$\sum_{i,i'} y_{ii'} = 1$$
, (4)

$$y_{ii'} \leq \lambda_i + \lambda_{i'} \forall i, i', (5)$$

$$0 \le \lambda_i \le 1 \forall i$$
, (6)

$$y_{ii'} \in \{0,1\} \forall i,i',(7)$$

## With metric constraint and investment category-specific budget constraint

$$\min_{y,\lambda} \sum_{i} \lambda_{i} q_{ik*}$$

subject to

 $\sum_{i} \sum_{j} \lambda_{i} c_{ij} \leq B$ , (1) Total budget constraint

 $\sum_{i} \lambda_{i} c_{ij'} \leq B_{j'} \forall j' \in J'$  (2) Investment category budget constraint(s)

 $\sum_{i} \lambda_{i} q_{ik'} \leq M_{k'}$ , (3) Metric constraint

$$\sum_{i} \lambda_i = 1$$
, (4)

$$\sum_{i,i'} y_{ii'} = 1$$
, (5)

$$y_{ii'} \leq \lambda_i + \lambda_{i'} \forall i, i', (6)$$

$$0 \le \lambda_i \le 1 \forall i$$
, (7)

$$y_{ii'} \in \{0,1\} \forall i,i',(8)$$

#### **Problem Size**

In general, I is the number of rows in the dataset of elicited data. In the case that all investment categories have elicited data at the same number of levels (not necessarily the same levels themselves), I can also be calculated as  $l^J$  where l is the number of investment levels.

The problem will involve  $\frac{I(I-1)}{2}$  binary variables and I continuous  $(\lambda)$  variables.

# 6.6 References

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6.6. References 49

# **PYTHON API**

The module tyche contains defines and solves multi-objective R&D optimization problems, which the module euty-chia provides a server of a web-based user interface. The module technology definies individual R&D technologies.

# 7.1 Tyche Module

## 7.1.1 tyche.DecisionGUI

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.

```
create_figure(i, j) \rightarrow Figure
```

mainloop()

Run the interactive interface.

**reevaluate** (next=<function Decision Window.<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.

```
{\tt refresh\_immediate} \ (\ )
```

Refresh the graphics immediately.

# 7.1.2 tyche.Designs

```
Designs for technologies.
class tyche.Designs.Designs(path=None, name='technology.xlsx', uncertain=True)
     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.

vectorize\_parameters (technology, scenario\_count, sample\_count=1)

Make an array of parameters.

vectorize\_scenarios (technology)

Make an array of scenarios.

vectorize\_technologies()

Make an array of technologies.

tyche.Designs.sampler(x, sample\_count)

Sample from an array.

#### **Parameters**

- **x** (array) The array.
- **sample\_count** (*int*) The sample size.

## 7.1.3 tyche.Distributions

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 *~numpy.random.Generator.choice* method of a *~numpy.random.Generator* instance instead; please see the 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 it 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. Default is True, meaning that a value of a can be selected multiple times.
- **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

7.1. Tyche Module 53

#### See also:

```
randint, shuffle, permutation
```

#### random.Generator.choice

which should be used in new code

#### **Notes**

Setting user-specified probabilities through p uses a more general but less efficient sampler than the default. The general sampler produces a different sample than the optimized sampler even if each element of p is 1 / len(a).

Sampling random rows from a 2-D array is not possible with this function, but is possible with *Generator.choice* through its axis keyword.

## **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.

# 7.1.4 tyche.EpsilonConstraints

Epsilon-constraint optimization.

```
class tyche.EpsilonConstraints.EpsilonConstraintOptimizer(evaluator, scale=1000000.0)
Bases: object
```

An epsilon-constration multi-objective optimizer.

#### evaluator

The technology evaluator.

### **Type**

tyche.Evaluator

#### scale

The scaling factor for output.

### **Type**

float

Maximize the objective function using the differential\_evoluaion algorithm.

#### **Parameters**

- **metric** (str) Name of metric to maximize. The objective function.
- sense (str) -

### Optimization sense ('min' or 'max'). If no value is provided to

this method, the sense value used to create the EpsilonConstraintOptimizer object is used instead.

- max\_amount (Series) Maximum investment amounts by R&D category. The index (research area) order must follow that of self.evaluator.max\_amount.index
- total\_amount (float) Upper limit on total investments summed across all R&D categories.
- **eps\_metric** (Dict) RHS of the epsilon constraint(s) on one or more metrics. Keys are metric names, and the values are dictionaries of the form {'limit': float, 'sense': str}. The sense defines whether the epsilon constraint is a lower or an upper bound, and the value must be either 'upper' or 'lower'.
- **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.

7.1. Tyche Module 55

- **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 and the differential\_evolution algorithm. verbose = 0 No messages verbose = 1 Objective function value at every algorithm iteration verbose = 2 Investment constraint status, metric constraint status, and objective function value verbose = 3 Decision variable values, investment constraint status, metric constraint status, and objective function value verbose > 3 All metric values, decision variable values, investment constraint status, metric constraint status, and objective function value

Maximize the objective function using a piecewise linear representation to create a mixed integer linear program.

#### **Parameters**

- **metric** (str) Name of metric to maximize
- **sense** (str) Optimization sense ('min' or 'max'). If no value is provided to this method, the sense value used to create the EpsilonConstraintOptimizer object is used instead.
- max\_amount (Series) Maximum investment amounts by R&D category. The index (research area) order must follow that of self.evaluator.max\_amount.index
- total\_amount (float) Upper limit on total investments summed across all R&D categories.
- **eps\_metric** (Dict) RHS of the epsilon constraint(s) on one or more metrics. Keys are metric names, and the values are dictionaries of the form {'limit': float, 'sense': str}. The sense defines whether the epsilon constraint is a lower or an upper bound, and the value must be either 'upper' or 'lower'.
- **statistic** (function) Summary statistic (metric measure) fed to evaluator\_corners\_wide method in Evaluator
- total\_amount Upper limit on total investments summed across all R&D categories
- **sizelimit** (*int*) Maximum allowed number of binary variables. If the problem size exceeds this limit, pwlinear\_milp will exit before building or solving the model.
- **verbose** (*int*) A value greater than zero will save the optimization model as a .lp file A value greater than 1 will print out status messages

### Returns

**Optimum** – exit\_code exit\_message amounts (None, if no solution found) metrics (None, if no solution found) solve\_time opt\_sense

#### Return type

NamedTuple

Maximize the objective function using the shgo global optimization algorithm.

#### **Parameters**

- metric (str) Name of metric to maximize.
- **sense** (str) Optimization sense ('min' or 'max'). If no value is provided to this method, the sense value used to create the EpsilonConstraintOptimizer object is used instead.
- max\_amount (Series) Maximum investment amounts by R&D category. The index (research area) order must follow that of self.evaluator.max\_amount.index
- total\_amount (float) Upper metric\_limit on total investments summed across all R&D categories.
- **eps\_metric** (Dict) RHS of the epsilon constraint(s) on one or more metrics. Keys are metric names, and the values are dictionaries of the form {'limit': float, 'sense': str}. The sense defines whether the epsilon constraint is a lower or an upper bound, and the value must be either 'upper' or 'lower'.
- **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. Defaults to None. Specifying this parameter can cause shoo to stall out instead of solving.
- **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 and the SHGO algorithm. verbose = 0 No messages verbose = 1 Convergence messages from SHGO algorithm verbose = 2 Investment constraint status, metric constraint status, and convergence messages verbose = 3 Decision variable values, investment constraint status, metric constraint status, and convergence messages verbose > 3 All metric values, decision variable values, investment constraint status, metric constraint status, and convergence messages

Optimize the objective function using the fmin\_slsqp algorithm.

### **Parameters**

- metric (str) Name of metric to maximize.
- **sense** (str) Optimization sense ('min' or 'max'). If no value is provided to this method, the sense value used to create the EpsilonConstraintOptimizer object is used instead.
- max\_amount (Series) Maximum investment amounts by R&D category. The index (research area) order must follow that of self.evaluator.max amount.index
- total\_amount (float) Upper limit on total investments summed across all R&D categories.
- **eps\_metric** (Dict) RHS of the epsilon constraint(s) on one or more metrics. Keys are metric names, and the values are dictionaries of the form {'limit': float, 'sense': str}. The

7.1. Tyche Module 57

sense defines whether the epsilon constraint is a lower or an upper bound, and the value must be either 'upper' or 'lower'.

- **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. Defaults to 0. verbose = 0 No messages verbose = 1 Summary message when fmin\_slsqp completes verbose = 2 Status of each algorithm iteration and summary message verbose = 3 Investment constraint status, metric constraint status, status of each algorithm iteration, and summary message verbose > 3 All metric values, decision variable values, investment constraint status, metric constraint status, status of each algorithm iteration, and summary message

Maximum value of metrics.

#### **Parameters**

- max\_amount (DataFrame) The maximum amounts that can be invested in each category.
- total\_amount (float) The maximum amount that can be invested in toto.
- **sense** (Dict or str) Optimization sense for each metric. Must be 'min' or 'max'. If None, then the sense provided to the EpsilonConstraintOptimizer class is used for all metrics. If string, the sense is used for all metrics.
- **statistic** (function) The statistic used on the sample evaluations.
- **tol** (*float*) The search tolerance.
- **maxiter** (*int*) The maximum iterations for the search.
- **verbose** (*int*) Verbosity level.

## 7.1.5 tyche.Evaluator

Fast evaluation of technology investments.

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

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\_corners\_semilong (statistic=<function mean>)

Return a dataframe indexed my investment amounts in each category, with columns for each metric.

#### **Parameters**

**statistic** (function) – The statistic to evaluate.

## evaluate\_corners\_wide (statistic=<function mean>)

Return a dataframe indexed my investment amounts in each category, with columns for each metric.

#### **Parameters**

**statistic** (function) – The statistic to evaluate.

#### evaluate\_statistic (amounts, statistic=<function mean>)

Evaluate a statistic for an investment.

#### **Parameters**

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

## make\_statistic\_evaluator(statistic=<function mean>)

Return a function that evaluates a statistic for an investment.

#### **Parameters**

**statistic** (function) – The statistic to evaluate.

7.1. Tyche Module 59

## 7.1.6 tyche.IO

I/O utilities for Tyche.

```
tyche.IO.check_tables(path, name)
```

Perform validity checks on input datasets.

All checks are run before this method terminates; that is, data errors are found all at once rather than one at a time from several calls to this method. A list of errors found is printed if any check fails. The errors include a summary of the check and identify the dataset that needs to be changed.

#### **Parameters**

- path (str) Path to directory of datasets
- name (str) Name of datasets file (XLSX)

#### Returns

**Boolean** 

## Return type

True if data is valid, False otherwise

## 7.1.7 tyche.Investments

Investments in technologies.

Bases: object

Investments in a technology.

### tranches

The *tranches* table.

## **Type**

DataFrame

#### investments

The investments table.

## Type

DataFrame

### compile()

Parse any probability distributions in the tranches.

```
evaluate_investments (designs, tranche_results=None, sample_count=1)
```

Evaluate the investments for a design.

- **designs** (tyche.Designs) The designs.
- **tranche\_results** (*tyche.Evaluations*) Output of evaluate\_tranches method. Necessary only if the investment amounts contain uncertainty.
- **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.
7.1.8 tyche. Types
Data types for Tyche.
class tyche.Types.Evaluations (amounts, metrics, summary, uncertain)
     Bases: tuple
     Named tuple type for rows in the evaluations table.
     amounts
          Alias for field number 0
     metrics
          Alias for field number 1
     summary
          Alias for field number 2
     uncertain
          Alias for field number 3
class tyche.Types.Functions(style, capital, fixed, production, metric)
     Bases: tuple
     Name tuple type for rows in the functions table.
     capital
          Alias for field number 1
     fixed
          Alias for field number 2
     metric
          Alias for field number 4
     production
          Alias for field number 3
     style
          Alias for field number 0
class tyche.Types.Indices(capital, input, output, metric)
```

Bases: tuple

capital

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

Alias for field number 0

7.1. Tyche Module 61

```
input
           Alias for field number 1
     metric
           Alias for field number 3
     output
          Alias for field number 2
class tyche.Types.Inputs (lifetime, scale, input, input_efficiency, input_price, output_efficiency, output_price)
     Bases: tuple
     Named tuple type for rows in the inputs table.
          Alias for field number 2
     input_efficiency
          Alias for field number 3
     input_price
          Alias for field number 4
     lifetime
           Alias for field number 0
     output_efficiency
          Alias for field number 5
     output price
           Alias for field number 6
     scale
           Alias for field number 1
class tyche.Types.Optimum(exit_code, exit_message, amounts, metrics, solve_time, opt_sense)
     Bases: tuple
     Named tuple type for optimization results.
     amounts
          Alias for field number 2
     exit_code
           Alias for field number 0
     exit_message
           Alias for field number 1
     metrics
          Alias for field number 3
     opt_sense
           Alias for field number 5
     solve_time
           Alias for field number 4
```

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

Bases: tuple

Named tuple type for rows in the results table.

cost

Alias for field number 0

metric

Alias for field number 2

output

Alias for field number 1

class tyche.Types.SynthesizedDistribution(rvs)

Bases: tuple

Named tuple type for a synthesized distribution.

rvs

Alias for field number 0

## 7.1.9 Module contents

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

# 7.2 Technology Module

# 7.2.1 Pre-Built Technology Models and Datasets

## **Residential Photovoltaics**

Generic model for residential PV.

This PV model tracks components, technologies, critical materials, and hazardous waste.

Table 7.1: Elements of capital arrays.

Index	Description	Units
0	module capital cost	\$/system
1	inverter capital cost	\$/system
2	balance capital cost	\$/system

Table 7.2: Elements of fixed arrays.

Index	Description	Units
0	fixed cost	\$/system

Table 7.3: Elements of input arrays.

Index	Description	Units
0	strategic metals	g/system

Table 7.4: Elements of output arrays.

Index	Description	Units
0	lifetime energy production	kWh/system
1	lifecycle hazardous waste	g/system
2	lifetime greenhouse gas production	gCO2e/system

Table 7.5: Elements of metric arrays.

Index	Description	Units
0	system cost	\$/Wdc
1	levelized energy cost	\$/kWh
2	greenhouse gas	gCO2e/kWh
3	strategic metal	g/kWh
4	hazardous waste	g/kWh
5	specific yield	hr/yr
6	module efficiency	%/100
7	module lifetime	yr

Table 7.6: Elements of parameter arrays.

Index	Description	Units
0	discount rate	1/yr
1	insolation	W/m^2
2	system size	m^2
3	module capital cost	\$/m^2
4	module lifetime	yr
5	module efficiency	%/100
6	module aperture	%/100
7	module fixed cost	\$/kW/yr
8	module degradation rate	1/yr
9	location capacity factor	%/100
10	module soiling loss	%/100
11	inverter capital cost	\$/W
12	inverter lifetime	yr
13	inverter replacement cost	%/100
14	inverter efficiency	%/100
15	hardware capital cost	\$/m^2
16	installation labor cost	\$/system
17	permitting cost	\$/system
18	customer acquisition cost	\$/system
19	installer overhead cost	%/100
20	hazardous waste content	g/m^2
21	greenhouse gas offset	gCO2e/kWh
22	benchmark LCOC	\$/Wdc
23	benchmark LCOE	\$/kWh

technology.pv\_residential\_large.capital\_cost (scale, parameter)
 Capital cost function.

## **Parameters**

• **scale** (*float*) – The scale of operation.

• parameter (array) – The technological parameterization.

technology.pv\_residential\_large.discount (rate, time)

Discount factor over a time period.

#### **Parameters**

- rate (float) The discount rate per time period.
- time (int) The number of time periods.

technology.pv\_residential\_large.fixed\_cost (scale, parameter)

Fixed cost function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- parameter (array) The technological parameterization.

technology.pv\_residential\_large.metrics(scale, capital, lifetime, fixed, input\_raw, input\_input\_price, output\_raw, output, cost, parameter)

Metrics function.

#### **Parameters**

- **scale** (float) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input\_raw (array) Raw input quantities (before losses).
- input (array) Input quantities.
- output\_raw (array) Raw output quantities (before losses).
- **output** (array) Output quantities.
- cost (array) Costs.
- parameter (array) The technological parameterization.

technology.pv\_residential\_large.module\_power(parameter)

Nominal module energy production.

#### **Parameters**

**parameter** (array) – The technological parameterization.

technology.pv\_residential\_large.npv (rate, time)

Net present value of constant cash flow.

### **Parameters**

- rate (float) The discount rate per time period.
- time (int) The number of time periods.

technology.pv\_residential\_large.performance\_ratio(parameter)

Performance ratio for the system.

#### Parameters

**parameter** (array) – The technological parameterization.

technology.pv\_residential\_large.production(scale, capital, lifetime, fixed, input, parameter)
Production function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input (array) Input quantities.
- parameter (array) The technological parameterization.

 $\verb|technology.pv_residential_large.specific_yield| (\textit{parameter})$ 

Specific yield for the system.

#### **Parameters**

**parameter** (array) – The technological parameterization.

## **Simple Residential Photovoltaics**

Simple residential PV.

technology.pv\_residential\_simple.capital\_cost (scale, parameter)
Capital cost function.

### **Parameters**

- **scale** (*float*) The scale of operation.
- **parameter** (array) The technological parameterization.

technology.pv\_residential\_simple.discount(rate, time)

Discount factor over a time period.

#### **Parameters**

- rate (float) The discount rate per time period.
- time (int) The number of time periods.

technology.pv\_residential\_simple.fixed\_cost(scale, parameter)

Fixed cost function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- **parameter** (array) The technological parameterization.

technology.pv\_residential\_simple.metrics (scale, capital, lifetime, fixed, input\_raw, input, input\_price, output\_raw, output, cost, parameter)

Metrics function.

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.

- **fixed** (array) Fixed costs.
- input\_raw (array) Raw input quantities (before losses).
- input (array) Input quantities.
- output\_raw (array) Raw output quantities (before losses).
- **output** (array) Output quantities.
- cost (array) Costs.
- parameter (array) The technological parameterization.

technology.pv\_residential\_simple.npv (rate, time)

Net present value of constant cash flow.

#### **Parameters**

- rate (float) The discount rate per time period.
- time (int) The number of time periods.

technology.pv\_residential\_simple.production(scale, capital, lifetime, fixed, input, parameter)

Production function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input (array) Input quantities.
- parameter (array) The technological parameterization.

## **Utility-Scale Photovoltaics**

Simple pv utility-scale module example. Inspired by Kavlak et al. Energy Policy 123 (2018) 700–710.

technology.utility\_pv.capital\_cost(scale, parameter)

Capital cost function.

### **Parameters**

- **scale** (*float*) The scale of operation.
- **parameter** (array) The technological parameterization.

technology.utility\_pv.fixed\_cost(scale, parameter)

Fixed cost function.

- **scale** (*float*) The scale of operation.
- parameter (array) The technological parameterization.

technology.utility\_pv.metrics(scale, capital, lifetime, fixed, input\_raw, input, input\_price, output\_raw, output, cost, parameter)

Metrics function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input\_raw (array) Raw input quantities (before losses).
- input (array) Input quantities.
- output\_raw (array) Raw output quantities (before losses).
- output (array) Output quantities.
- cost (array) Costs.
- parameter (array) The technological parameterization.

technology.utility\_pv.production(scale, capital, lifetime, fixed, input, parameter)

Production function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input (array) Input quantities.
- **parameter** (array) The technological parameterization.

## **Transportation**

Phase-1 model to estimate the cost, energy, and emissions associated with a particular vehicle/transport technology.

```
technology.transport_model.capital_cost(scale, parameter)
```

Capital cost function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- parameter (array) The technological parameterization.

technology.transport\_model.fixed\_cost (scale, parameter)

Capital cost function.

- **scale** (*float*) The scale of operation.
- parameter (array) The technological parameterization.

technology.transport\_model.metrics(scale, capital, lifetime, fixed, input\_raw, input\_price, output raw, output, cost, parameter)

Metrics function.

#### **Parameters**

- scale (float) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input\_raw (array) Raw input quantities (before losses).
- input (array) Input quantities.
- output\_raw (array) Raw output quantities (before losses).
- output (array) Output quantities.
- cost (array) Costs.
- **parameter** (array) The technological parameterization.

technology.transport\_model.production(scale, capital, lifetime, fixed, input, parameter)

Production function.

#### **Parameters**

- scale (float) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input (array) Input quantities.
- **parameter** (array) The technological parameterization.

# 7.2.2 Tutorial Technologies

The technology models in this section are for exploratory and learning purposes only.

#### Simple Electrolysis

Simple electrolysis.

technology.simple\_electrolysis.capital\_cost (scale, parameter)
Capital cost function.

- **scale** (*float*) The scale of operation.
- parameter (array) The technological parameterization.

technology.simple\_electrolysis.fixed\_cost (scale, parameter)

Fixed cost function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- parameter (array) The technological parameterization.

technology.simple\_electrolysis.metrics(scale, capital, lifetime, fixed, input\_raw, input\_price, output\_raw, output, cost, parameter)

Metrics function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input\_raw (array) Raw input quantities (before losses).
- input (array) Input quantities.
- output\_raw (array) Raw output quantities (before losses).
- **output** (array) Output quantities.
- cost (array) Costs.
- parameter (array) The technological parameterization.

technology.simple\_electrolysis.production(scale, capital, lifetime, fixed, input, parameter)

Production function.

### **Parameters**

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input (array) Input quantities.
- parameter (array) The technological parameterization.

### **Toy Biorefinery**

Biorefinery model with four processing steps.

technology.tutorial\_biorefinery.capital\_cost (scale, parameter)
Capital cost function.

- **scale** (*float*) The scale of operation.
- parameter (array) The technological parameterization.

#### Return type

Total capital cost for one biorefinery (USD/biorefinery)

technology.tutorial\_biorefinery.fixed\_cost (scale, parameter)

Fixed cost function.

#### **Parameters**

- scale (float [Unused]) The scale of operation.
- **parameter** (array) The technological parameterization.

#### Return type

total fixed costs for one biorefinery (USD/year)

technology.tutorial\_biorefinery.metrics (scale, capital, lifetime, fixed, input\_raw, input\_price, output\_raw, output, cost, parameter)

Metrics function.

#### **Parameters**

- scale (float) The scale of operation. Unitless
- capital (array) Capital costs. Units: USD/biorefinery
- lifetime (float) Technology lifetime. Units: year
- fixed (array) Fixed costs. Units: USD/year
- input\_raw (array) Raw input quantities (before losses). Units: metric ton feed-stock/year
- input (array) Input quantities. Units: metric ton feedstock/year
- input\_price (array`) Array of input prices. Various units.
- output\_raw (array) Raw output quantities (before losses). Units: gal biofuel/year
- output (array) Output quantities. Units: gal biofuel/year
- cost (array) Costs.
- parameter (array) The technological parameterization. Units vary; given in comments below

technology.tutorial\_biorefinery.production (scale, capital, lifetime, fixed, input, parameter)

Production function.

#### **Parameters**

- scale (float) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- fixed (array) Fixed costs.
- input (array) Input quantities.
- parameter (array) The technological parameterization.

#### Returns

Ideal/theoretical production of each technology output: biofuel at gals/year

### Return type

output\_raw

### **Onshore Wind Turbines**

Template for technology functions.

```
technology.tutorial_basic.capital_cost(scale, parameter)
```

Capital cost function.

#### **Parameters**

- scale (float) The scale of operation.
- **parameter** (array) The technological parameterization.

technology.tutorial\_basic.fixed\_cost(scale, parameter)

Capital cost function.

### **Parameters**

- **scale** (*float*) The scale of operation.
- **parameter** (array) The technological parameterization.

technology.tutorial\_basic.metrics(scale, capital, lifetime, fixed, input\_raw, input\_input\_price, output\_raw, output, cost, parameter)

Metrics function.

#### **Parameters**

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input raw (array) Raw input quantities (before losses).
- input (array) Input quantities.
- **output\_raw** (array) Raw output quantities (before losses).
- output (array) Output quantities.
- cost (array) Costs.
- **parameter** (array) The technological parameterization.

technology.tutorial\_basic.production(scale, capital, lifetime, fixed, input, parameter)

Production function.

- **scale** (*float*) The scale of operation.
- capital (array) Capital costs.
- lifetime (float) Technology lifetime.
- **fixed** (array) Fixed costs.
- input (array) Input quantities.
- **parameter** (array) The technological parameterization.

# 7.2.3 Module contents

# **PYTHON MODULE INDEX**

# t technology, 73 technology.pv\_residential\_large,63 technology.pv\_residential\_simple,66 technology.simple\_electrolysis,69 technology.transport\_model,68 technology.tutorial\_basic,72 technology.tutorial\_biorefinery,70 technology.utility\_pv,67 tyche, 63 tyche.DecisionGUI, 51 tyche.Designs, 52 tyche.Distributions, 53 tyche.EpsilonConstraints,55 tyche.Evaluator, 58 tyche. Investments, 60 tyche. IO, 60 tyche. Types, 61