Tyche

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

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

TYCHE QUICK START GUIDE

1.1 Introduction and Getting Started

1.1.1 Set up Tyche package

There are several platforms for using Tyche. Listed below is the process of downloading the Tyche framework to your personal computer. The Tyche repository is available on github at this [link](https://github.com/NREL/tyche). A library of simple Tyche models is available at to provide beginning templates for developing more complete models of technologies of interest [here.](https://github.com/NREL/tyche/tree/dev/src/technology)

- Download and install [Anaconda](https://www.anaconda.com/). No need for installing Anaconda for Linux or Mac systems.

- Download Tyche from GitHub

- Navigate to the downloaded Tyche repository folder.

- **Create the Tyche environment**

    - Type the following into the Anaconda Shell (under Anaconda in the Windows Start menu). For Mac use system terminal.

    - Windows OS: `conda env create --file conda\win.yml `

    - Mac OS: `conda env create --file conda\mac.yml `

    - `conda activate tyche`

    - `pip install mip`

1.1.2 Repository Organization

The directory where users should store new technology models (.py files) and the accompanying datasets (discussed below) is indicated in blue. We recommend that users create sub-directories under technology for each new technology or decision context, to avoid confusing the various input datasets.

1.2 Defining a Technology Model

1.2.1 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 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, 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 classic but simple and generalized techno-economic analysis (TEA). The TEA is based on a user defined technology model and accompanying datasets of technological and investment information.

1.3 Input Datasets

1.3.1 Designs Dataset

A *design* is one set of technology data that results from a specific R&D investment scenario. The *designs* dataset collects the technologies and technology versions that may result from all R&D investment scenarios being considered in a decision context.

The *designs* dataset contains information for one or more technologies being compared within an R&D investment decision context. There will be multiple sets of data for each technology; each set represents the technology data that results from a specific R&D investment scenario. Tables 2 and 3 provide a data dictionary for the *designs* dataset.

Table 1:

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	- Input - Input efficiency - Input price - Output efficiency - Output price - Lifetime - Scale	Variable types required by technology model and related functions.
Index	String	Any	Name of the elements within each Variable.
Value	- Float - Distribution - Mixture of distributions	- 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.

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 break the code. The Value for irrelevant Variables may be set to 0 or 1. Variables and their component Indexes are defined further in Table 2.

Table 2:

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

1.3.2 Parameters Dataset

The *parameters* dataset contains any ad hoc data, other than that contained in the *designs* dataset, that is required to calculate a technology's capital cost, fixed cost, production (actual output amount(s)), and metrics. If the information in the *designs* dataset completely defines the technology and its metrics of interest, then the *parameters* dataset can be left blank except for the column names. Identically to the *designs* dataset, the *parameters* dataset contains multiple sets of data corresponding to different R&D investment scenarios.

Table 3:

Column Name	Data type	Description
Technology	String	Name of the technology.
Scenario	String	Name of the R&D investment scenario that resulted in the corresponding parameter values or distributions.
Parameter	String	Name of the parameter.
Offset	String	Numerical location of the parameter.
Value	Float; Distribution; Mixture of distributions	Parameter value for the R&D investment scenario. Example: st.triang(1,loc=5,scale=0.1)
Units	String	Parameter units. User defined; not used or checked during Tyche calculations.
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.

1.3.3 Technology model Python 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 4 describes methods that must be included in the technology model Python file. The names of the methods are user-defined and must match the contents of the *functions* dataset, discussed below. Additional methods can be included in the technology model, if necessary, but the methods in Table 4 are required. All return values for the required methods must be formatted as numpy "stacks" of values; for more information, see the numpy documentation.

Table 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.＿

Recom-mended Method Name	Parameters	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) output amount(s).
metrics	scale, capital, lifetime, fixed, input_raw, input, input_price, output_raw, output, cost, parameter	Calculated technology metric 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*).

1.4 Defining R&D Investments

1.4.1 Tranches Dataset

A *tranche* is a discrete unit of R&D investment (dollar amount) in a specific research category. 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 the allowed 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 using expert elicitation. A data dictionary for the *tranches* dataset is given in Table 5.

Table 5:

Column Name	Data Type	Description
Category	String	Names of the R&D categories in which investment can be made to impact the technology or technologies being studied.
Tranche	String	Names of the tranches.
Scenario	String	Names of the R&D investment scenarios, which combine tranches across R&D categories. The names in this column must correspond to the Scenarios listed in the designs and parameters datasets.
Amount	Float; Distribution; Mixture of distributions	The R&D investment amount of the Tranche. The amount may be defined as a scalar, a probability distribution, or a mix of probability distributions.
Notes	String	Additional user-defined information. Not used by Tyche.

1.4.2 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 6.

Table 6:

Column Name	Data Type	Description
Investment	String	Name of the R&D investment. Distinct from the Scenarios.
Category	String	Names of the R&D categories being invested in. Within each row, the Category must match the Tranche.
Tranche	String	Names of the tranches within the Investment. Within each row, the Tranche must match the Category
Notes	String Additional user-defined information. Not used by Tyche.

1.5 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.

1.5.1 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](https://docs.scipy.org/doc/scipy/reference/stats.html) 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.

1.6 Additional Input Datasets

1.6.1 Indices Dataset

The *indices* dataset contains the numerical indexes (location within a list or array) used to access content in the other datasets. Table 7 describes the columns required for the indices table. Numerical locations for parameters should not be listed in this dataset.

Table 7:

Column Name	Data Type	Allowed Values	Description
Technology	String	Any	Name of the technology
Type	String	- Capital - Input - Output - Metric	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.

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.

1.6.2 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.

1.6.3 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 4. Table 8 provides a data dictionary for the *functions* dataset.

Table 8:

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

The Style should remain *numpy* in Tyche 1.0. 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.

1.6.4 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 9.

Table 9:

Column Name	Data Type	Allowed Values	Description
Technology	String	Any	Name of the technology.
Variable	String	- Cost - Output - Metric	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.

The Variable "Cost" is a technology-wide lifetime cost, and as such may not be relevant within all decision contexts. To fill in the Index values for the "Output" and "Metric" Variables, see the *designs* dataset.

APPROACH

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

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

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

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

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

MATHEMATICAL FORMULATION

We separate the financial and conversion-efficiency aspects of a production process, which are generic across all technologies, from the physical and technical aspects, which are necessarily specific to the particular process. The motivation for this is that the financial and waste computations can be done uniformly for any technology (even for disparate ones such as PV cells and biofuels) and that different experts may be required to assess the cost, waste, and techno-physical aspects of technological progress. Table 3.1 defines the indices that are used for the variables that are defined in Table 3.2.

Table 3.1: 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 3.2: Definitions for variables.

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

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Table 3.2 – continued from previous page

Variable	Type	Description	Units
P_o	function	production function	output/unit
M_m	function	metric function	metric/unit
α_p	parameter	technical parameter	(mixed)
ξ_θ	variable	scenario inputs	(mixed)
ζ_θ	variable	scenario outputs	(mixed)
ψ	function	scenario evaluation	(mixed)
σ_ϕ	function	scenario probability	1
q_ϕ	variable	investment cost	USD
ζ_ϕ	random variable	investment outcome	(mixed)
$\mathbf{Z}(\omega)$	random variable	portfolio outcome	(mixed)
$Q(\omega)$	calculated	portfolio cost	USD
$Q^{\min}$	parameter	minimum portfolio cost	USD
$Q^{\max}$	parameter	maximum portfolio cost	USD
$q_\phi^{\min}$	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)
$\mathbb{F}, \mathbb{G}$	operator	evaluate probabilities	(mixed)

3.1 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:

$$K = \left(\sum_c C_c / \tau_c + \sum_f F_f \right) / S + \sum_i p_i \cdot I_i - \sum_o p'_o \cdot O_o$$

3.2 Waste

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

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

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

3.3 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.

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

3.4 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.

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

3.5 Scenarios

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

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

and the tuple of output variables

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

and their relationship

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

given the tuple of functions

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

for the technology of the scenario.

3.6 Investments

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

$$\sigma_\phi(\theta) = P\left(\theta|\phi\right).$$

such that

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

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

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

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

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

The cost of an investment in one of the constituents ϕ is q_ϕ, so the cost of a porfolio is:

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

3.7 Decision problem

The multi-objective decision problem is

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

such that

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

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

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

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

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

3.8 Experts

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

ELECTROLYSIS EXAMPLE

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

$H_2O \rightarrow H_2 + \frac{1}{2} O_2$
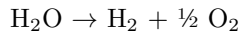
Experts could assess how much R&D to increase the various efficiencies η would cost. They could also suggest different catalysts, adding alkali, or replacing the process with PEM.

4.1 Tracked quantities.

$\mathcal{C} = \{\text{catalyst}\}$

$\mathcal{F} = \{\text{rent}\}$

$\mathcal{I} = \{\text{water}, \text{electricity}\}$

$\mathcal{O} = \{\text{oxygen}, \text{hydrogen}\}$

$\mathcal{M} = \{\text{cost}, \text{GHG}, \text{jobs}\}$

4.2 Current design.

$I_{\text{water}} = 19.04$ g/mole

$\eta_{\text{water}} = 0.95$ (due to mass transport loss on input)

$I_{\text{electricity}} = 279$ kJ/mole

$\eta_{\text{electricity}} = 0.85$ (due to ohmic losses on input)

$\eta_{\text{oxygen}} = 0.90$ (due to mass transport loss on output)

$\eta_{\text{hydrogen}} = 0.90$ (due to mass transport loss on output)

4.3 Current costs.

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

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

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

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

4.4 Current prices.

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

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

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

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

4.5 Production function (à la Leontief)

$P_{\text{oxygen}} = (16.00 \text{ g}) \cdot \min \left\{ \frac{I^*_{\text{water}}}{18.08 \text{ g}}, \frac{I^*_{\text{electricity}}}{237 \text{ kJ}} \right\}$

$P_{\text{hydrogen}} = (2.00 \text{ g}) \cdot \min \left\{ \frac{I^*_{\text{water}}}{18.08 \text{ g}}, \frac{I^*_{\text{electricity}}}{237 \text{ kJ}} \right\}$

4.6 Metric function.

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

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

$M_{\text{jobs}} = (0.00015 \text{ job/mole}) / O_{\text{hydrogen}}$

4.7 Performance of current design.

$K = 0.18 \text{ USD/mole}$ (i.e., not profitable since it is positive)

$O_{\text{oxygen}} = 14 \text{ g/mole}$

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

$\mu_{\text{cost}} = 0.102 \text{ USD/gH2}$

$\mu_{\text{GHG}} = 21.4 \text{ gCO2e/gH2}$

$\mu_{\text{jobs}} = 0.000083 \text{ job/gH2}$

DATABASE SCHEMA

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

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

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

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

5.1 Metadata about indices

The `indices` table (see Table 5.1) simply describes the various indices available for the variables. The `Offset` column specifies the memory location in the argument for the production and metric functions.

Table 5.1: 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	

5.2 Design variables

The `design` table (see Table 5.2) specifies the values of all of the variables in the mathematical formulation of the design. Note that the `Value` column can either contain numeric literals or Python expressions specifying probability distribution functions. For example, a normal distribution with mean of five and standard deviation of two would be written `st.norm(5, 2)`. All of the Scipy probability distribution functions are available for use, as are two special functions, `constant` and `mixture`. The `constant` distribution is just a single constant value; the `mixture` distribution is the mixture of a list of distributions, with specified relative weights. The `mixture` function is particularly important because it allows one to specify a first distribution in the case of an R&D breakthrough, but a second distribution if no breakthrough occurs.

Table 5.2: Example of the `designs` table.

Technology	Scenario	Variable	Index	Value	Units	Notes
Simple electrolysis	Base	Input	Water	19.04	g/mole	I_{water}
Simple electrolysis	Base	Input Efficiency	Water	0.95	1	η_{water}
Simple electrolysis	Base	Input	Electricity	279	kJ/mole	$I_{\text{electricity}}$
Simple electrolysis	Base	Input Efficiency	Electricity	0.85	1	$\eta_{\text{electricity}}$
Simple electrolysis	Base	Output Efficiency	Oxygen	0.90	1	η_{oxygen}
Simple electrolysis	Base	Output Efficiency	Hydrogen	0.90	1	η_{hydrogen}
Simple electrolysis	Base	Lifetime	Catalyst	3	yr	τ_{catalyst}
Simple electrolysis	Base	Scale		6650	mole/yr	S
Simple electrolysis	Base	Input price	Water	4.8e-3	USD/mole	p_{water}
Simple electrolysis	Base	Input price	Electricity	3.33e-5	USD/kJ	$p_{\text{electricity}}$
Simple electrolysis	Base	Output price	Oxygen	3.0e-3	USD/g	p_{oxygen}
Simple electrolysis	Base	Output price	Hydrogen	1.0e-2	USD/g	p_{hydrogen}

5.3 Metadata for functions

The `functions` table (see Table 5.3) simply documents which Python module and functions to use for the technology and scenario. Currently only the `numpy` style of function is supported, but later `plain` Python functions and `tensorflow` functions will be allowed.

Table 5.3: Example of the `functions` table.

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

5.4 Parameters for functions

The `parameters` table (see Table 5.4) contains ad-hoc parameters specific to the particular production and metrics functions. The `Offset` column specifies the memory location in the argument for the production and metric functions.

Table 5.4: Example of the `parameters` table.

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

5.5 Units for results

The `results` table (see Table 5.5) simply specifies the units for the results.

Table 5.5: Example of the `results` table.

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

5.6 Tranches of investments.

In the `tranches` table (see Table 5.6), each *category* of investment contains a set of mutually exclusive *tranches* that may be associated with one or more *scenarios* defined in the `designs` table. Typically, a category is associated with a technology area and each tranche corresponds to an investment strategy within that category.

Table 5.6: Example of the `tranches` table.

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

5.7 Investments

In the `investments` table (see Table 5.7), each *investment* is associated with a single *tranche* in one or more *categories*. An investment typically combines tranches from several different investment categories.

Table 5.7: Example of the `investments` table.

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

DEFINING TECHNOLOGIES

Each technology design requires a Python module with a capital cost, a fixed cost, a production, and a metrics function. Listing 6.1 shows these functions for the simple electrolysis example.

Listing 6.1: Example technology-defining functions.

```python
# Simple electrolysis.


# All of the computations must be vectorized, so use `numpy`.
import numpy as np


# Capital-cost function.
def capital_cost(
  scale,
  parameter
):

  # Scale the reference values.
  return np.stack([np.multiply(
    parameter[6], np.divide(scale, parameter[5])
  )])


# Fixed-cost function.
def fixed_cost(
  scale,
  parameter
):

  # Scale the reference values.
  return np.stack([np.multiply(
    parameter[7],
    np.divide(scale, parameter[5])
  )])


# Production function.
def production(
  capital,
```

```python
  fixed,
  input,
  parameter
):

  # Moles of input.
  water       = np.divide(input[0], parameter[2])
  electricity = np.divide(input[1], parameter[3])

  # Moles of output.
  output = np.minimum(water, electricity)

  # Grams of output.
  oxygen   = np.multiply(output, parameter[0])
  hydrogen = np.multiply(output, parameter[1])

  # Package results.
  return np.stack([oxygen, hydrogen])


# Metrics function.
def metrics(
  capital,
  fixed,
  input_raw,
  input,
  img/output_raw,
  output,
  cost,
  parameter
):

  # Hydrogen output.
  hydrogen = output[1]

  # Cost of hydrogen.
  cost1 = np.divide(cost, hydrogen)

  # Jobs normalized to hydrogen.
  jobs = np.divide(parameter[4], hydrogen)

  # GHGs associated with water and electricity.
  water       = np.multiply(input_raw[0], parameter[8])
  electricity = np.multiply(input_raw[1], parameter[9])
  co2e = np.divide(np.add(water, electricity), hydrogen)

  # Package results.
  return np.stack([cost1, jobs, co2e])
```

OPTIMIZATION

7.1 Non-Linear (NLP) Formulation Summary

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

- Ability to perform constrained optimization with inequality constraints

- Ability to optimize without specified Jacobian or Hessian functions

- Ability to specify bounds on individual decision variables

- Ability to work on a variety of potentially non-convex and otherwise complex problems

7.1.1 Solutions to `pv_residential_simple`

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

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

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	•

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

7.2 Sequential Least Squares Programming

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

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

Maximize the objective function using the `fmin_slsqp` algorithm.

Parameters

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

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

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

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

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

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

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

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

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

Return

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

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

7.2.1 Defining Constraints

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

7.2.2 SLSQP Solution to `pv_residential_simple`

Solve time: 1.5 s

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

System Metric	Optimized Value
GHG	41.97
LCOE	0.038
Labor	0.032

7.3 Differential Evolution

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

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

Parameters

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

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

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

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

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

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

`seed` [int] Sets the random seed for optimization by creating a new `RandomState` instance. Defaults to 2 for reproducible solutions. If a value is not provided, then `differential_evolution` will return slightly different solutions for the same optimization problem every time it is called.

`init` [str or array-like] Type of population initialization. Defaults to 'latinhypercube'. Alternative initializations are 'random' (which does not guarantee good coverage of the solution space) or specifying every member of the initial population in an array of shape (`popsize`, `len(variables)`). The latter option is useful when the global minimum is known to be in a small portion of the solution space, and the initialization can seed the population in this area. However, this parameter is not analogous to specifying initial values for decision variables, as each candidate solution in the population must be unique for the algorithm to optimize correctly.

`tol` [float] Relative tolerance for convergence, which provides an upper limit on the standard deviation of candidate solutions. When this upper limit is met, the optimization has converged. Defaults to 0.01. The convergence tolerance for this algorithm was loosened compared to the other algorithms to lessen the execution time and increase the changes of the algorithm converging. Tighter tolerances (lower values of `tol`) tended to prevent the algorithm converging.

maxiter [int] Upper limit on generations of candidate solution evolution, which corresponds to the number of algorithm iterations. Each iteration involves many function evaluations as each solution in the population evolves. Defaults to 75.

verbose [int] Verbosity level returned by this outer function and the differential_evolution algorithm. Defaults to 0. * 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.

Returns

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

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

7.3.1 Defining Constraints

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

7.3.2 Differential Evolution Solutions to `pv_residential_simple`

Solution 1

- Seed = 2

- Solve time = 145 s

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

System Metric	Optimized Value
GHG	41.70
LCOE	0.038
Labor	-0.456

Solution 2

- Seed = 1

- Solve time = 589

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

System Metric	Optimized Value
GHG	41.63
LCOE	0.037
Labor	-2.29

7.4 Simplicial Homology Global Optimization

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

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

Maximize the objective function using the shgo global optimization algorithm.

Parameters

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

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

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

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

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

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

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

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

verbose [int] Verbosity level returned by this outer function and the SHGO algorithm. Defaults to 0. * 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 .

Returns

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

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

7.4.1 Defining Constraints

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

```
constraints = [ {'type': 'ineq', 'fun': g1(x)},
                {'type': 'ineq', 'fun': g2(x)},
                ...
                {'type': 'eq', 'fun': h1(x)},
                {'type': 'eq', 'fun': h2(x)},
                ... ]
```

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

7.5 Piecewise Linear (MILP) Formulation Summary

7.5.1 Notation

Table 7.1: 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 7.2: Data definitions for the MILP formulation.

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

Table 7.3: Variable definitions for the MILP formulation.

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

Each metric and investment amount can be written as a linear combination of elicited data points and the newly introduced variables λ_i and $y_{ii'}$. Additional constraints on $y_{ii'}$ and λ_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.

7.5.2 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 λ 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 λ 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 λ 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 λ and y variables.)

7.5.3 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) $0 \leq \lambda_i \leq 1 \forall i$, (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) $0 \leq \lambda_i \leq 1 \forall i$, (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) $0 \leq \lambda_i \leq 1 \forall i$, (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 (λ) variables.

7.6 References

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6. Kraft D (1988) A software package for sequential quadratic programming. Tech. Rep. DFVLR-FB 88-28, DLR German Aerospace Center — Institute for Flight Mechanics, Koln, Germany.

7. `scipy.optimize.NonlinearConstraint` SciPy v1.5.4 Reference Guide: Optimization and root finding (`scipy.optimize`) URL: https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.NonlinearConstraint.html Last accessed 12/29/2020.

USER INTERFACE

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

1. **Focused analysis** comparing investment scenarios to examine impact across metrics when exploring options during the decision-making process and

2. **Broader communication** of Office goals externally, such as through the dissemination of a funding opportunity announcement.

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

8.1 User Input

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

1. Balance of System R&D

2. Inverter R&D

3. Module R&D

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

Metrics A user can also select up to three metrics to impact through R&D on these selected investment categories and specify goals that must be met. The current options include:

1. Greenhouse gas emissions (ΔgCO2e/system)

2. Labor (Δ\$/system)

3. Levelized cost of energy (Δ\$/kWh)

8.2 Modes

The Eutychia interface operates in two modes:

1. **Explore Mode**, checked by default,

2. **Optimize Mode**, which can be enabled by deselecting "explore." Entering Optimize Mode allows users to update optimization parameters.

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

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

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

8.3 Visualizations

Users are presented with the option to interact with the data in varying levels of detail. These options are enabled to suit the needs of users, from those who prefer a snapshot of the bigger picture for quick analysis to those who would like to study the distributional probability of achieving each metric. Plots are generated using the Seaborn 0.11.0 package.[1] The available visualizations in order of increasing level of detail include:

1. **Heatmaps** (`heatmap`) with metric scaled to percent of the maximum possible improvement,

2. **Annotated heatmaps** with metric values overlayed, and

3. **Distributions** with the probability of ahieving each metric based on the number of samples. At this stage of development, these results can be viewed in columns (by metric) or in a grid. The user can select from the following options:

   - Box plots (`boxplot`)

   - Probability distributions (`kdeplot`)

   - Violin plots (`violinplot`)

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

8.4 References

---

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

TUTORIAL

Multiple Objectives for Residential PV.

9.1 Import packages.

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

```python
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
```

9.2 Load data.

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

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

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

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

```python
designs.compile()
```

9.3 Examine the data.

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

```python
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
```

9.4 Evaluate the scenarios in the dataset.

```
scenario_results = designs.evaluate_scenarios(sample_count=50)
```

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

9.4.1 Save results.

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

9.4.2 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"        ,
```

(continues on next page)

```
        "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);
```
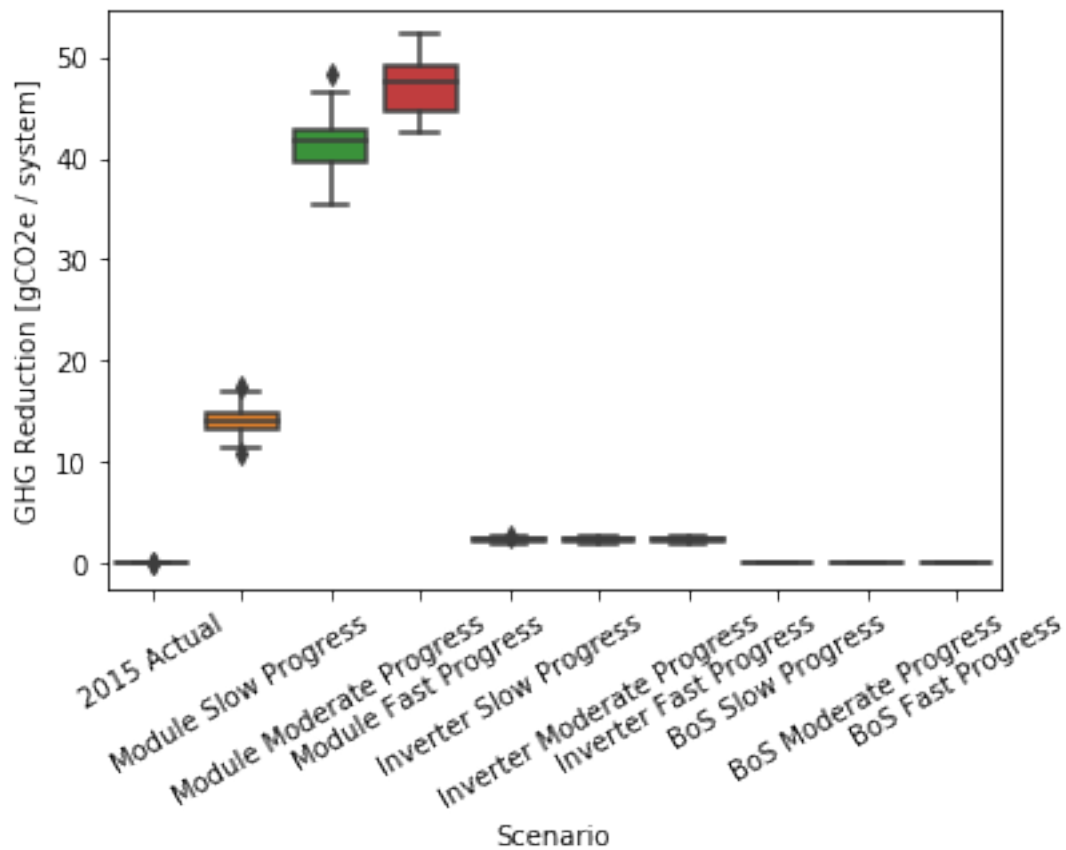

9.4.3 Plot LCOE metric.

```
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);
```


9.4.4 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);
```
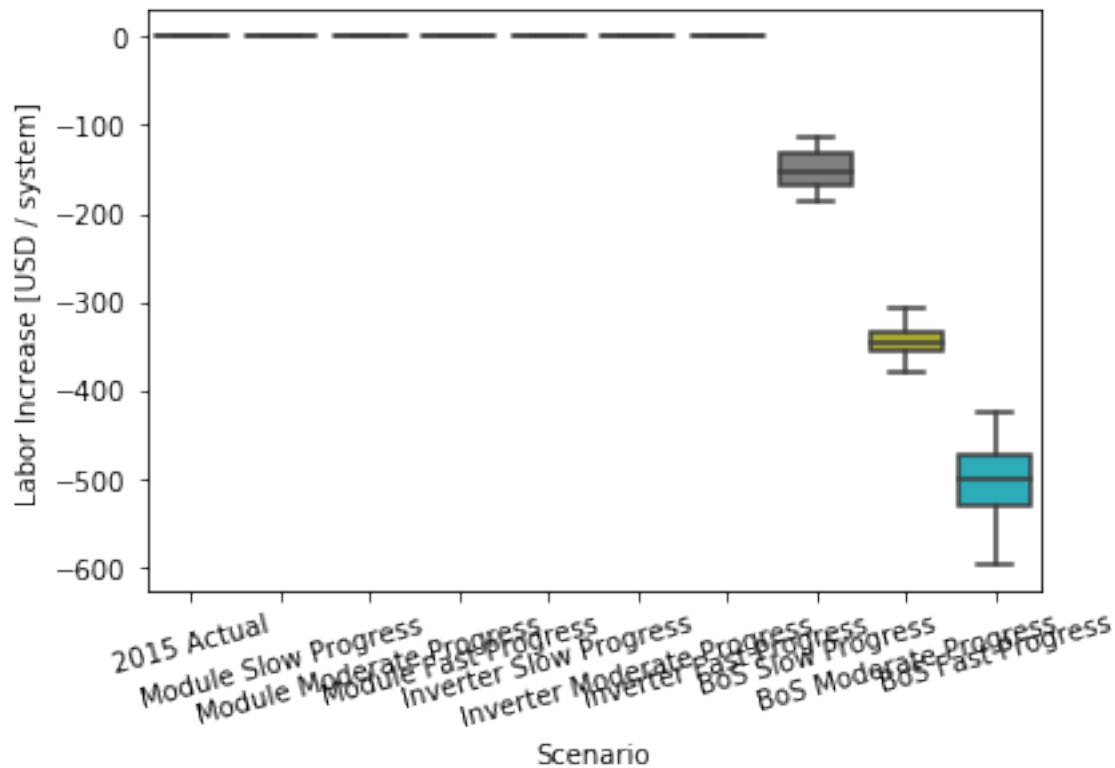

9.5 Evaluate the investments in the dataset.

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

9.5.1 Costs of investments.

```
investment_results.amounts
```

9.5.2 Benefits of investments.

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

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

9.5.3 Save results.

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

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

9.5.4 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);
```
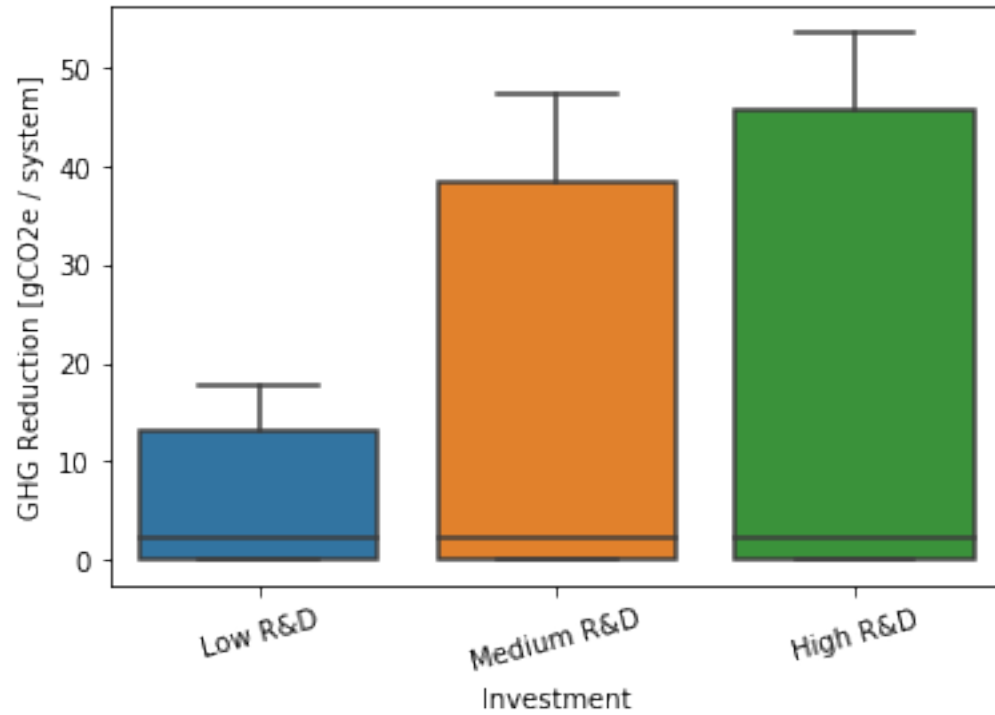
9.5.5 Plot LCOE metric.

```
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);
```
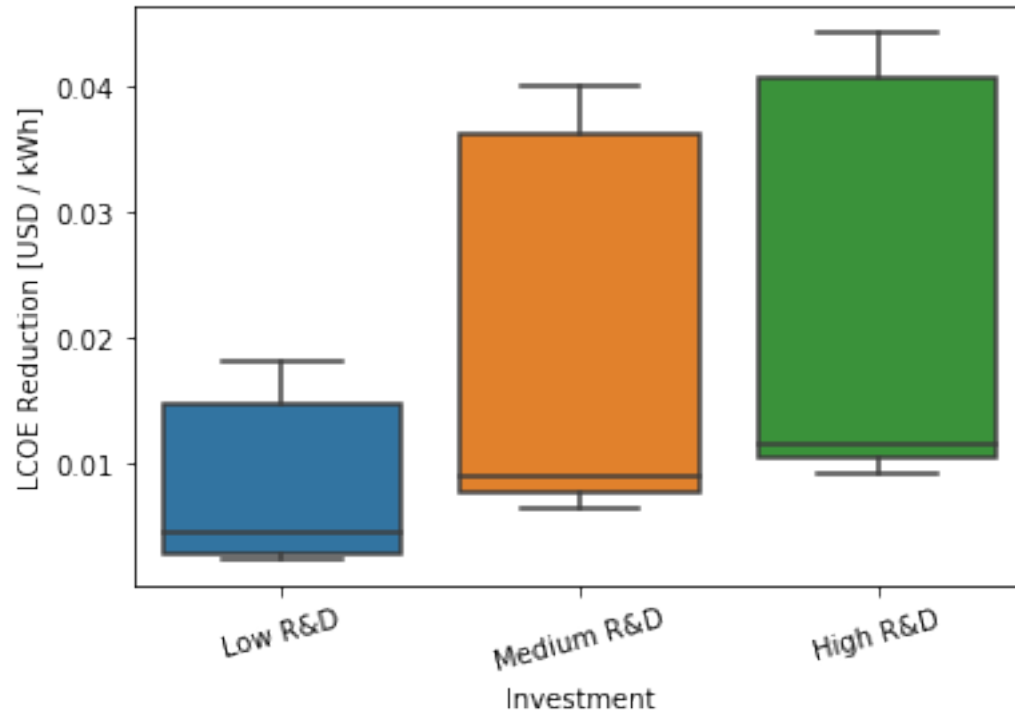
9.5.6 Plot labor metric.

```
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);
```
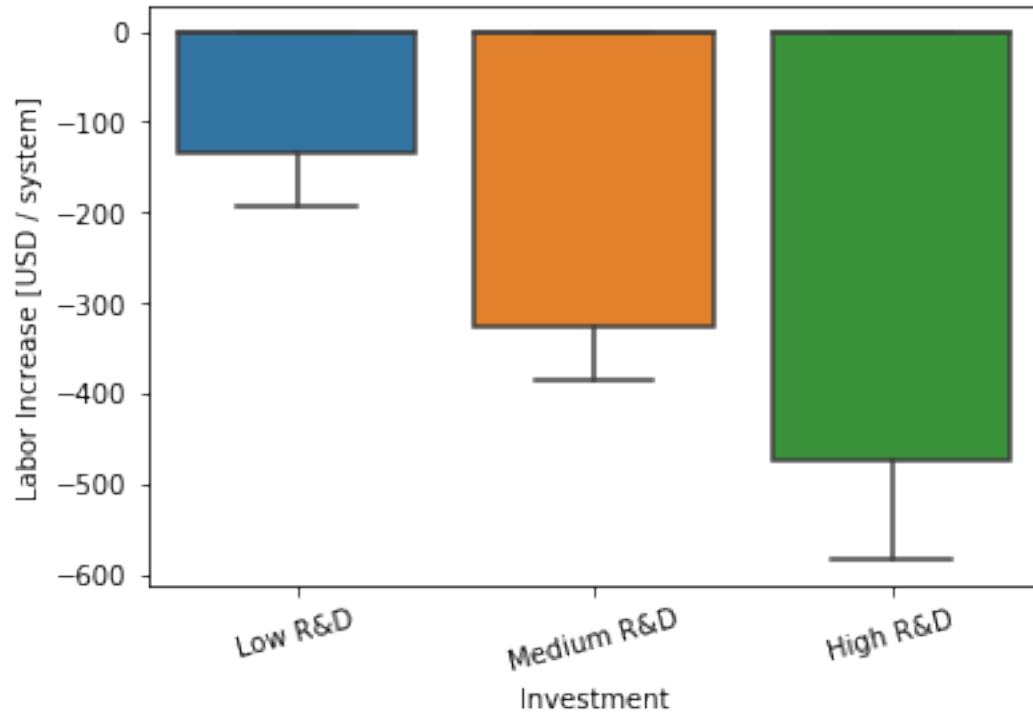
9.6 Multi-objective decision analysis.

9.6.1 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.

```
tranche_results.amounts.to_csv("output/pv_residential_simple/example-tranche-amounts.csv
↪")
tranche_results.summary.to_csv("output/pv_residential_simple/example-tranche-summary.csv
↪")
```

9.6.2 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
```

9.6.2.1 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    1         -0.0010586097518157094
                    2          7.493162517135921e-05
                    3          0.001253893601450784
                    4         -0.00398626797827717
                    5         -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
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
```

9.6.3 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
```

9.6.3.1 Example optimization.

Limit spending to $3M.

```
investment_max = 3e6
```

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

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

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

Compute the ϵ-constrained maximum for the LCOE.

```
optimum = optimizer.maximize(
    "LCOE"                          ,
    total_amount = investment_max,
    min_metric   = metric_min     ,
    statistic    = np.mean        ,
)
optimum.exit_message
```

```
'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.

```
optimum = optimizer.maximize(
    "LCOE"                              ,
    total_amount = investment_max,
    min_metric   = metric_min     ,
    statistic    = lambda x: np.quantile(x, 0.1),
)
optimum.exit_message
```

```
'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"]),
```

<div align="right">(continues on next page)</div>

```
    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
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
```

9.6.4 Pareto surfaces.

9.6.4.1 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
```

```
sb.relplot(
    x         = "Investment [M$]",
    y         = "Value"          ,
    col       = "Metric"         ,
    kind      = "line"           ,
    facet_kws = {'sharey': False},
    data      = pareto_amounts.reset_index().melt(id_vars = "Investment [M$]", var_name␣
↪= "Metric", value_name = "Value")
)
```

```
<seaborn.axisgrid.FacetGrid at 0x7f9da11752b0>
```
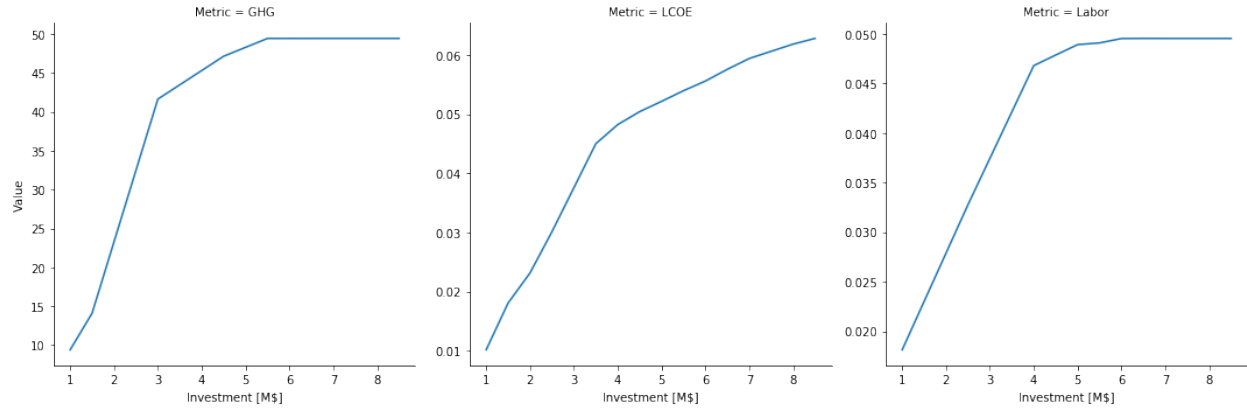
We see that the LCOE metric saturates more slowly than the GHG and Labor ones.

9.6.4.2 GHG vs LCOE, constrained by total investment.

```python
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
```

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

```python
<seaborn.axisgrid.FacetGrid at 0x7f9da13ae630>
```
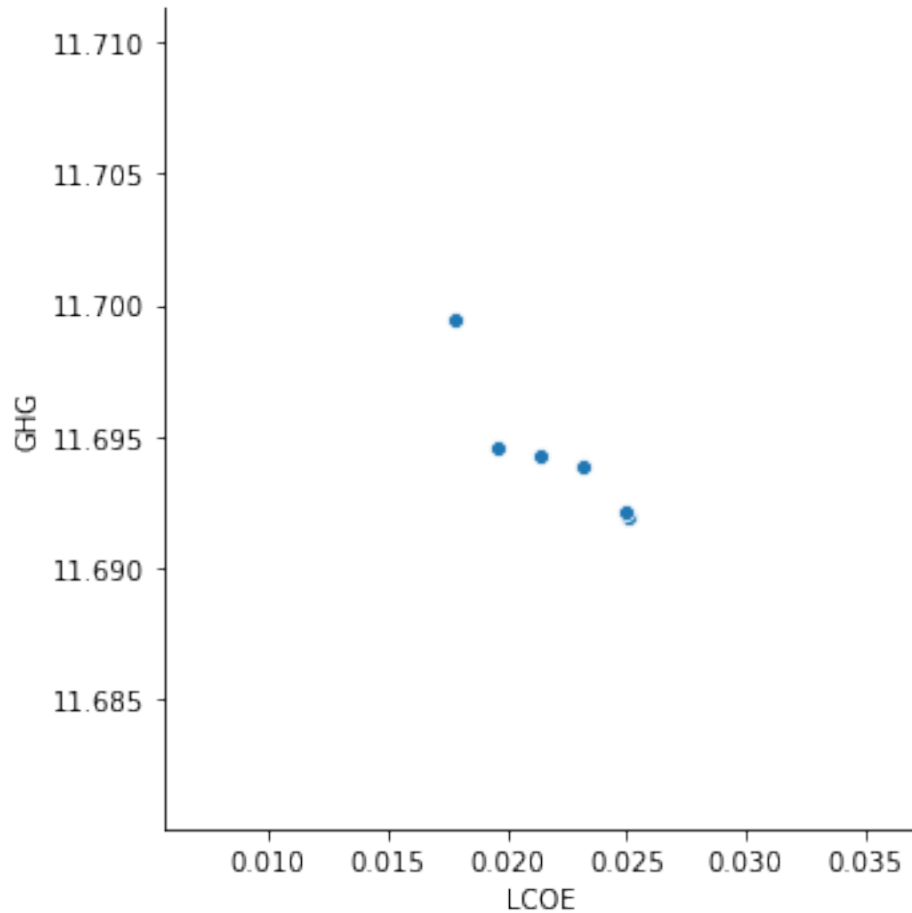
The three types of investment are too decoupled to make an interesting pareto frontier, and we also need a better solver if we want to push to lower right.

9.7 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")
```
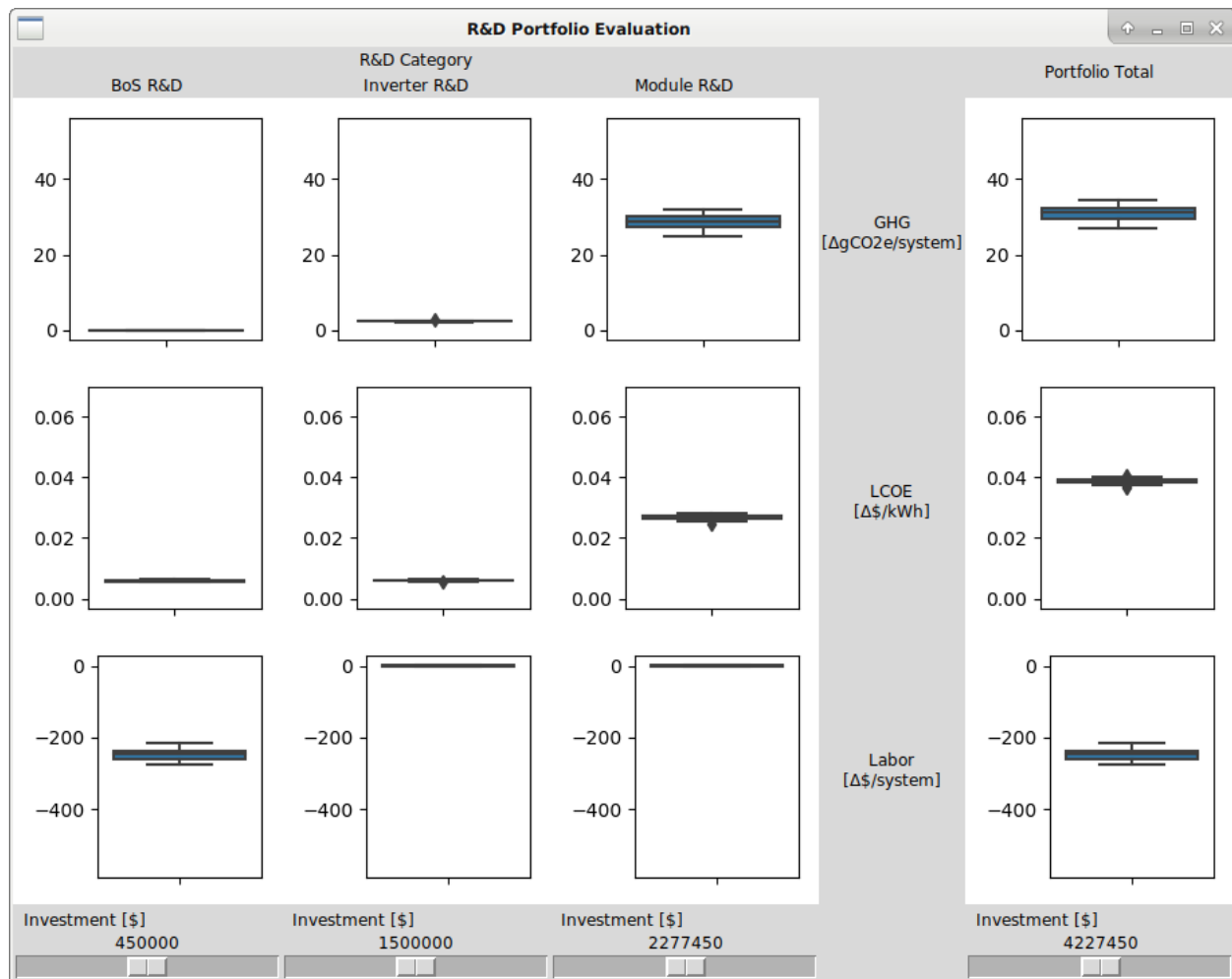
MOCK FOA DEFINITION

10.1 Background

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

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

10.1.1 Phases

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

1. **Launch**. Decide to issue a FOA.

2. **Frame**. Formulate a plan to collect the information necessary to write the FOA

3. **Scope**. Investigate topic options.

4. **Draft**. Compile information into draft FOA.

5. **Refine**. Prepare FOA for distribution.

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

10.1.2 Roles

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

- Technical analyst

- Technical lead

- FOA lead

- Approver

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

10.2 Potential topics

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

Topics under consideration might be assessed by the following metrics:

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

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

10.2.1 1. Crystaline silicon wafer design

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

10.2.2 2. Tandem thin-films

- Design parameters
- Architectures

10.2.3 3. Polysilicon module

- (many parameters)

10.2.4 4. Module design

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

10.2.5 5. Inverter design

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

10.2.6 6. Balance-of-system design

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

MOCK FOA EXAMPLE

11.1 Set up.

11.1.1 Import packages.

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

```python
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
```

11.2 Load data.

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

```python
designs = ty.Designs("data")
```

```python
investments = ty.Investments("data")
```

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

```python
designs.compile()
```

11.3 Examine the input data.

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

```python
designs.functions
```

The `indices` table defines the subscripts for variables.

```
designs.indices.drop("Offset", axis = 1)
```

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

```
designs.designs.xs("Reference", level = "Scenario", drop_level = False)
```

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

```
designs.parameters.drop("Offset", axis = 1).xs("Reference", level = "Scenario", drop_
↪level = False)
```

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
```

11.4 Evaluate the scenarios in the dataset.

```
scenario_results = designs.evaluate_scenarios(sample_count=500)
```

Format results as a pivot table.

```
scenario_results.xs(
    "PV Generic"
).groupby(
    ["Scenario", "Variable", "Index"]
).aggregate(
    np.mean
).xs(
    "Metric", level = 1
).pivot_table(
    index = "Scenario", columns = "Index"
)
```

Print the units for the columns.

```
designs.results.loc["PV Generic", "Metric"].transpose()
```

11.5 Save results.

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

11.5.1 Plot the results.

```
g = sb.FacetGrid(
    data = investments.tranches.join(scenario_results).xs("Metric", level = "Variable").
↪reset_index(),
    row = "Category",
    col = "Index",
    sharex = False,
    sharey = False,
)
g.map(
    sb.violinplot,
    "Value",
    "Tranche",
)
```

/nix/store/2hqyq1p29z76wvh920r43a63sy9n1cag-python3-3.7.6-env/lib/python3.7/site-
↪packages/seaborn/axisgrid.py:728: UserWarning: Using the violinplot function without␣
↪specifying *order* is likely to produce an incorrect plot.
  warnings.warn(warning)

```
<seaborn.axisgrid.FacetGrid at 0x7f93daf77d10>
```

11.6 Evaluate the investments in the dataset.

```
investment_results = investments.evaluate_investments(designs, sample_count=500)
```

11.6.1 Costs of investments.

```
investment_results.amounts
```

11.6.2 Benefits of investments.

```
investment_results.summary.set_index(
    "Units", append = True
).groupby(
    ["Investment", "Index", "Units"]
).aggregate(
    np.mean
).pivot_table(
    index = ["Index", "Units"],
    columns = "Investment",
)
```

11.6.3 Save results.

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

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

11.6.4 Plot the results.

```
investment_results.summary
```

```
g = sb.FacetGrid(
    data = investment_results.summary.reset_index(),
    col = "Index",
    sharex = False,
    col_wrap = 4
)
g.map(
    sb.violinplot,
    "Value",
    "Investment",
)
```

```
/nix/store/2hqyq1p29z76wvh920r43a63sy9n1cag-python3-3.7.6-env/lib/python3.7/site-
→packages/seaborn/axisgrid.py:728: UserWarning: Using the violinplot function without␣
→specifying order is likely to produce an incorrect plot.
  warnings.warn(warning)
```

```
<seaborn.axisgrid.FacetGrid at 0x7f93dafe6750>
```
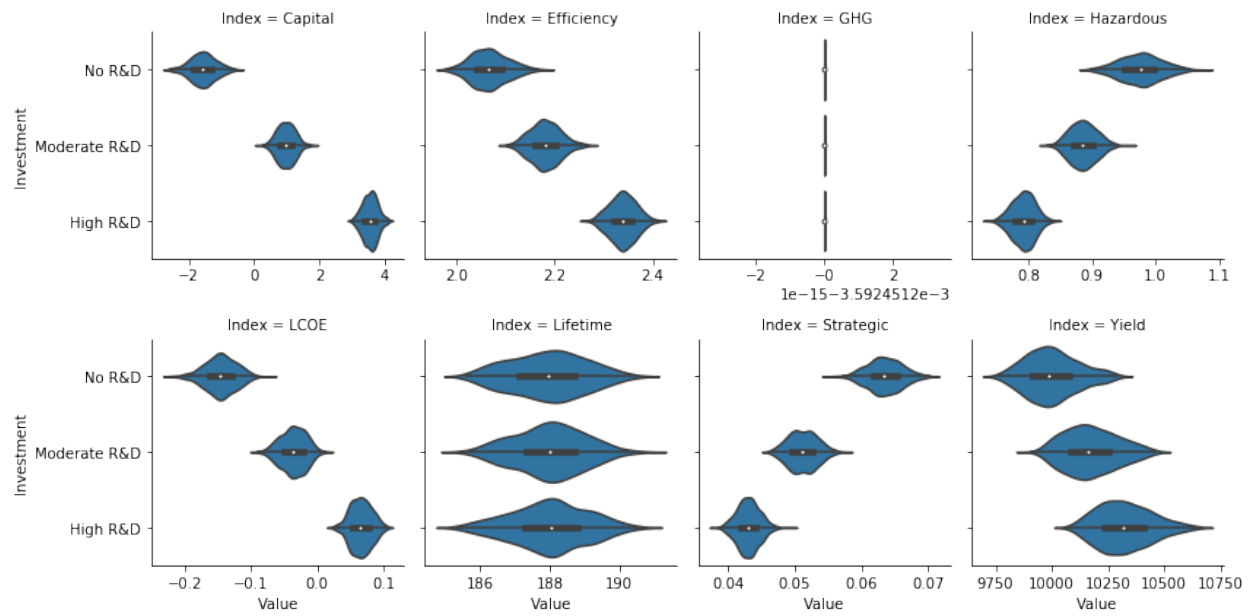
DEPLOYMENT PLAN

12.1 Objectives

1. Securely house all potentially sensitive data within on DOE servers within the DOE intranet.

2. Minimize the deployment and maintenance burden at DOE.

3. Assure the quality of software and data updates.

4. Enable DOE personnel and contractors to contribute technology models and data.

12.2 Components and Activities
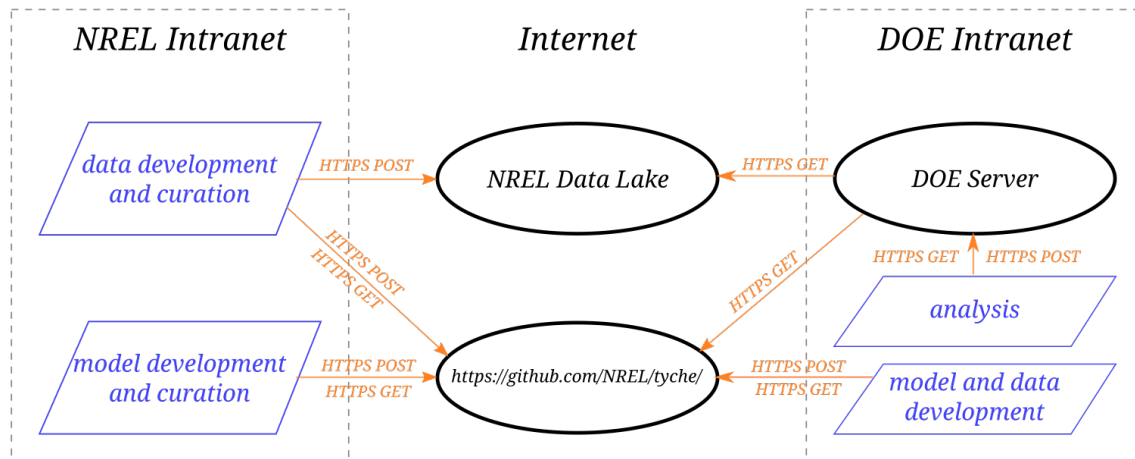
Fig. 12.1: Deployment of services and activities.

12.3 Activities

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

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

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

12.4 Components

12.4.1 DOE Server

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

1. Linux (preferred) or Windows.

2. Four to 16 CPU cores and at least 32 GB of memory.

3. An up-to-date installation (version 4.8.3 or later) of the Conda software package manager.

4. Installation of the Tyche environment within Conda. (This will install the correct version of Python and the other required software, so those need not be installed individually.) See the attachment conda-environment.yml.

5. Running a shell script for the Quart HTTP server.

6. Open outgoing HTTPS ports for `GET` requests to the NREL Data Lake and GitHub.com.

7. An open HTTP incoming port from client web browsers withing the DOE intranet.

8. A folder on disk that is regularly backed up.

12.4.2 NREL Data Lake

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

12.4.3 GitHub Software Repository

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

12.5 Security Considerations

1. NREL has authority to operate (ATO) with non-sensitive software and data on its Data Lake and on GitHub.com.

2. Sensitive data (in the form of scenario definitions and results) may reside on the DOE server and on the laptops of DOE users.

3. The Tyche service only makes HTTPS `GET` requests outside of the DOE intranet, and these only consist of fetching non-sensitive datasets and technology models. Thus, the firewall for the Tyche server should be configured at follows:

    1. Block all incoming traffic from outside the DOE intranet.

    2. Allow incoming HTTP traffic from inside the DOE intranet.

    3. Allow outgoing HTTPS traffic to NREL Data Lake and GitHub.com.

    4. Block all other outgoing traffic.

4. Ideally, the Tyche software (and its library dependencies) and its updates should undergo a security audit.

GETTING STARTED

Instruction for Running the Example and the Server

13.1 Conda Environment

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

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

on Windows, or on Mac

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

If you receive an HTTPS error, consider retrying the command with the *–insecure* flag added. Note that the conda environment was created with the command:

```
conda create -n tyche -c conda-forge python=3.7 numpy scipy scikit-learn seaborn=0.10␣
→matplotlib=3.3 quart hypercorn jupyter
```

13.2 Running the Server

Visit the folder **src/eutychia/** and start the server in debug mode

```
cd src\eutychia
debug.cmd
```

on Windows, or on Mac

```
cd src/eutychia
./debug.sh
```

or in production mode

```
cd src\eutychia
run.cmd
```

on Windows, or on Mac

```
cd src/eutychia
./run.sh
```

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

13.3 Running the Example

Using Jupyter, first start the notebook server

```
jupyter notebook
```

and visit http://localhost:8888/ to select `example.ipynb` in the folder `src/eutychia`.

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

PYTHON API

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

14.1 tyche package

14.1.1 Submodules

14.1.2 tyche.DecisionGUI module

Interactive exploration of a technology.

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

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

> **create_figure**(*i*, *j*) → matplotlib.figure.Figure

> **mainloop()**
> > Run the interactive interface.

> **reevaluate**(*next=<function DecisionWindow.<lambda>>*, *delay=200*)
> > Recalculate the results after a delay.

> > **Parameters**

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

> **reevaluate_immediate**(*next=<function DecisionWindow.<lambda>>*)
> > Recalculate the results immediately.

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

> **refresh()**
> > Refresh the graphics after a delay.

> **refresh_immediate()**
> > Refresh the graphics immediately.

14.1.3 tyche.Designs module

Designs for technologies.

class tyche.Designs.**Designs**(*path=None,   indices='indices.csv',   functions='functions.csv',   designs='designs.csv',   parameters='parameters.csv',   results='results.csv'*)

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.

14.1.4 tyche.Distributions module

Utilities for probability distributions.

tyche.Distributions.choice(*a*, *size=None*, *replace=True*, *p=None*)
> Generates a random sample from a given 1-D array

> New in version 1.7.0.

> **Note:** New code should use the **choice** method of a **default_rng()** instance instead; 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 a were np.arange(a)

>>> - **size** (*int or tuple of ints, optional*) – Output shape. If the given shape is, e.g., (m, n, k), then m * n * k samples are drawn. Default is None, in which case a single value is returned.

>>> - **replace** (*boolean, optional*) – Whether the sample is with or without replacement

>>> - **p** (*1-D array-like, optional*) – The probabilities associated with each entry in a. If not given the sample assumes a uniform distribution over all entries in a.

>> **Returns samples** – The generated random samples

>> **Return type** single item or ndarray

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

> **See also:**

> **randint()**, **shuffle()**, **permutation()**

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

> ### Notes

> 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:

```
>>> aa_milne_arr = ['pooh', 'rabbit', 'piglet', 'Christopher']
>>> np.random.choice(aa_milne_arr, 5, p=[0.5, 0.1, 0.1, 0.3])
array(['pooh', 'pooh', 'pooh', 'Christopher', 'piglet'], # random
      dtype='<U11')
```

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.

14.1.5 tyche.EpsilonConstraints module

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

opt_diffev(*metric*, *sense=None*, *max_amount=None*, *total_amount=None*, *eps_metric=None*,
>   *statistic=<function mean>*, *strategy='best1bin'*, *seed=2*, *tol=0.01*, *maxiter=75*,
>   *init='latinhypercube'*, *verbose=0*)
>   Maximize the objective function using the differential_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** (*DataFrame*) – Maximum investment amounts by R&D category (de-
>>>>   fined in investments data) and maximum metric values

>>> -   **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.

>>> -   **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 differen-
>>>>   tial_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 val-
>>>>   ues, 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

opt_milp(*metric*, *sense=None*, *max_amount=None*, *total_amount=None*, *eps_metric=None*, *statistic=<function mean>*, *sizelimit=1000000.0*, *verbose=0*)
> 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** (*DataFrame*) – Maximum investment amounts by R&D category (defined in investments data) and maximum metric values

> - **total_amount** (*float*) – Upper limit on total investments summed across all R&D categories.

> - **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

opt_shgo(*metric*, *sense=None*, *max_amount=None*, *total_amount=None*, *eps_metric=None*, *statistic=<function mean>*, *tol=0.01*, *maxiter=None*, *sampling_method='simplicial'*, *verbose=0*)
> 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** (*DataFrame*) – Maximum investment amounts by R&D category (defined in investments data) and maximum metric values

> - **total_amount** (*float*) – Upper metric_limit on total investments summed across all R&D categories.

> - **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 evalua-
  tions; 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 shgo 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 al-
  gorithm. 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 met-
  ric values, decision variable values, investment constraint status, metric constraint
  status, and convergence messages

opt_slsqp(*metric*, *sense=None*, *max_amount=None*, *total_amount=None*, *eps_metric=None*,
      statistic=<function mean>, *initial=None*, *tol=1e-08*, *maxiter=50*, *verbose=0*)
    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** (*DataFrame*) – Maximum investment amounts by R&D category (de-
  fined in investments data) and maximum metric values

- **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.

- **initial** (*array of float*) – Initial value of decision variable(s) fed to the opti-
  mizer.

- **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

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

class tyche.EpsilonConstraints.**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

14.1.6 tyche.Evaluator module

Fast evaluation of technology investments.

class tyche.Evaluator.**Evaluator**(*tranches*, *summary*)
  Bases: `object`

  Evalutate technology investments using a response surface.

  amounts
    Cost of tranches.

      Type DataFrame

  categories
    Categories of investment.

Type DataFrame

metrics
> Metrics for technologies.
>> **Type** DataFrame

units
> Units of measure for metrics.
>> **Type** DataFrame

interpolators
> Interpolation functions for technology metrics.
>> **Type** DataFrame

evaluate(*amounts*)
> Sample the distribution for an investment.
>> **Parameters amounts** (*DataFrame*) – The investment levels.

evaluate_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 valuates a statistic for an investment.
>> **Parameters statistic** (*function*) – The statistic to evaluate.

14.1.7 tyche.IO module

I/O utilities for Tyche.

tyche.IO.make_table(*dtypes*, *index*)
> Make a data frame from column types and an index.
>> **Parameters**
>> - **dtypes** (*array*) – The column types.
>> - **index** (*array*) – The index.

tyche.IO.read_table(*path*, *name*, *dtypes*, *index*)
> Read a data table from a file.
>> **Parameters**

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

14.1.8 tyche.Investments module

Investments in technologies.

class tyche.Investments.**Investments**(*path=None*,   *tranches='tranches.csv'*,   *investments='investments.csv'*)

Bases: `object`

Investments in a technology.

tranches
> The *tranches* table.
>
> > **Type** DataFrame

investments
> The *investments* table.
>
> > **Type** DataFrame

evaluate_investments(*designs*, *sample_count=1*)
> Evaluate the investments for a design.
>
> > **Parameters**
> >
> > - **designs** (*tyche.Designs*) – The designs.
> > - **sample_count** (*int*) – The number of random samples.

evaluate_tranches(*designs*, *sample_count=1*)
> Evaluate the tranches of investment for a design.
>
> > **Parameters**
> >
> > - **designs** (*tyche.Designs*) – The designs.
> > - **sample_count** (*int*) – The number of random samples.

14.1.9 tyche.Types module

Data types for Tyche.

class tyche.Types.**Evaluations**(*amounts*, *metrics*, *summary*)
Bases: `tuple`

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

amounts
> Alias for field number 0

metrics
> Alias for field number 1

summary
> Alias for field number 2

class tyche.Types.**FakeDistribution**(*rvs*)

    Bases: `tuple`

    Named tuple type for a fake distribution.

    rvs

        Alias for field number 0

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

    Bases: `tuple`

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

    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`

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

    capital

        Alias for field number 0

    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.

    input

        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.**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

14.1.10 Module contents

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

14.2 eutychia package

14.2.1 Submodules

14.2.2 eutychia.example module

Example script for multiple objective optimization of residential PV.

14.2.3 eutychia.main module

14.2.4 Module contents

Eutychia: user interface for a Python package for R&D pathways analysis and evaluation.

14.3 Technology Module

14.3.1 Technology Case Studies

14.3.1.1 Residential Photovoltaics

Generic model for residential PV.

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

Table 14.1: Elements of `capital` arrays.

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

Table 14.2: Elements of `fixed` arrays.

Index	Description	Units
0	fixed cost	$/system

Table 14.3: Elements of `input` arrays.

Index	Description	Units
0	strategic metals	g/system

Table 14.4: 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 14.5: 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 14.6: 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.

technology.pv_residential_large.**specific_yield**(*parameter*)
   Specific yield for the system.

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

14.3.1.2 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.

> > **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_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.

14.3.1.3 Utiliy-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.

>> **Parameters**

>>> - **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.

14.3.1.4 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.

        Parameters

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

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

`technology.transport_model.`**`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.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.

14.3.2 Tutorial Technologies

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

14.3.2.1 Toy Biorefinery

Biorefinery model with four processing steps.

`technology.tutorial_biorefinery.`**`capital_cost`**(*scale*, *parameter*)
    Capital cost function.

> **Parameters**
>
> > - **scale** (*float*) – The scale of operation.
> > - **parameter** (*array*) – The technological parameterization.
>
> **Returns**
>
> **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.
>
> **Returns**
>
> **Return type** total fixed costs for one biorefinery (USD/year)

`technology.tutorial_biorefinery.`**`metrics`**(*scale*, *capital*, *lifetime*, *fixed*, *input_raw*, *input*, *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 feedstock/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

14.3.2.2 Simple Electrolysis

Simple electrolysis.

technology.simple_electrolysis.**capital_cost**(*scale*, *parameter*)
　　Capital cost function.

Parameters

- **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*, *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.

14.3.2.3 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.

> > **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.

14.3.3 Module contents

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