desdeo_problem

Release 1.0

Multiobjective Optimization Group

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CONTENTS

Contains tools to model and define multiobjective optimization problems to be used in the DESDEO framework.

CHAPTER

ONE

REQUIREMENTS

- Python 3.7 or newer.
- Poetry dependency manager : Only for developers.

See *pyproject.toml* for Python package requirements.

CHAPTER

TWO

INSTALLATION

To install and use this package on a *nix-based system, follow one of the following procedures.

2.1 For users

First, create a new virtual environment for the project. Then install the package using the following command:

```
$ pip install desdeo_problem
```

2.2 For developers

Download the code or clone it with the following command:

```
$ git clone https://github.com/industrial-optimization-group/desdeo-problem
```

Then, create a new virtual environment for the project and install the package in it:

```
$ cd desdeo-problem
$ poetry init
$ poetry install
```

2.2.1 API Documentation

desdeo_problem.problem Package

Desdeo-problem package

This package is for creating a problem for desdeo to solve. It includes modules for Variables, Objectives, Constraints, and actual Problem.

Functions

constraint_function_factory(lhs, rhs, operator)	A function that creates an evaluator.
variable_builder(names, initial_values[, ...])	Automatically build all variable objects.

constraint_function_factory

desdeo_problem.problem.**constraint_function_factory**(*lhs*, *rhs*, *operator*)

A function that creates an evaluator.

This function creates an evaluator to be used with the ScalarConstraint class. Constraints should be formulated in a way where all the mathematical expression are on the left hand side, and the constants on the right hand side.

Parameters

- **lhs** (*Callable*) – The left hand side of the constraint. Should be a callable function representing a mathematical expression.
- **rhs** (*float*) – The right hand side of a constraint. Represents the right hand side of the constraint.
- **operator** (*str*) – The kind of constraint. Can be '==', '<', '>'.

Returns A function that can be called to evaluate the rhs and which returns representing how the constraint is obeyed. A negative value represent a violation of the constraint and a positive value an agreement with the constraint. The absolute value of the float is a direct indicator how the constraint is violated/agdreed with.

Return type Callable

Raises **ValueError** – The supplied operator is not supported.

variable_builder

desdeo_problem.problem.**variable_builder**(*names*, *initial_values*, *lower_bounds=None*, *upper_bounds=None*)

Automatically build all variable objects.

Parameters

- **names** (*List[str]*) – Names of the variables
- **initial_values** (*np.ndarray*) – Initial values taken by the variables.
- **lower_bounds** (*Union[List[float], np.ndarray], optional*) – Lower bounds of the variables. If None, it defaults to negative infinity. Defaults to None.
- **upper_bounds** (*Union[List[float], np.ndarray], optional*) – Upper bounds of the variables. If None, it defaults to positive infinity. Defaults to None.

Raises ***VariableError*** – Lengths of the input arrays are different.

Returns List of variable objects

Return type List[*Variable*]

Classes

ScalarConstraint(name, n_decision_vars, ...)	A simple scalar constraint that evaluates to a single scalar.
ConstraintError	Raised when an error related to the Constraint class in encountered.
ConstraintBase()	Base class for constraints.
ObjectiveBase()	The abstract base class for objectives.
ObjectiveError	Raised when an error related to the Objective class is encountered.
ObjectiveEvaluationResults(objectives, ...)	The return object of <problem>.evaluate methods.
VectorObjectiveBase()	The abstract base class for multiple objectives which are calculated at once.
ScalarObjective(name, evaluator[, ...])	A simple objective function that returns a scalar.
_ScalarObjective(name, evaluator[, ...])	
VectorObjective(name, evaluator[, ...])	An objective object that calculated one or more objective functions.
ScalarDataObjective(name, data[, evaluator, ...])	A simple Objective class for single valued objectives.
_ScalarDataObjective(name, data[, ...])	
VectorDataObjective(name, data[, evaluator, ...])	A Objective class for multi/valued objectives.
ProblemError	Raised when an error related to the Problem class is encountered.
ProblemBase()	The base class for the problems.
EvaluationResults(objectives, fitness, ...)	The return object of <problem>.evaluate methods.
ScalarMOProblem(objectives, variables, ...)	A multiobjective optimization problem.
ScalarDataProblem(decision_vectors, ...)	A problem class for case where the data is precomputed.
MOProblem(objectives, variables[, ...])	An user defined multiobjective optimization problem.
DataProblem(data, variable_names, ...[, ...])	A class for a data based problem.
ExperimentalProblem(variable_names, ...[, ...])	A problem class for data-based problem.
VariableError	Raised when an error is encountered during the handling of the Variable objects.
VariableBuilderError	Raised when an error is encountered during the handling of the Variable objects.
Variable(name, initial_value[, lower_bound, ...])	Simple variable with a name, initial value and bounds.
DiscreteDataProblem(data, variable_names, ...)	A problem class for data-based problems with discrete values.
classificationPISProblem(objectives, ...[, ...])	A problem class for the IOPIS formulation for interactive optimization.

ScalarConstraint

class desdeo_problem.problem.**ScalarConstraint**(*name*, *n_decision_vars*, *n_objective_funs*, *evaluator*)

Bases: desdeo_problem.problem.Constraint.ConstraintBase

A simple scalar constraint that evaluates to a single scalar.

Parameters

- **name** (*str*) – Name of the constraint.
- **n_decision_vars** (*int*) – Number of decision variables present in the constraint.
- **n_objective_funs** (*int*) – Number of objective functions present in the constraint.
- **evaluator** (*Callable*) – A callable to evaluate the constraint.

__name
Name of the constraint.

Type str

__n_decision_vars
Number of decision variables present in the constraint.

Type int

__n_objective_funs
Number of objective functions present in the constraint.

Type int

__evaluator
A callable to evaluate the constraint.

Type Callable

Attributes Summary

evaluator	constraint evaluator callable
n_decision_vars	number of decision variables
n_objective_funs	number of objective functions
name	name

Methods Summary

evaluate(decision_vector, objective_vector)	Evaluate the constraint.

Attributes Documentation

evaluator
constraint evaluator callable

Returns A callable to evaluate the constraint.

Return type Callable

Type Property

n_decision_vars
number of decision variables

Returns Number of decision variables

Return type int

Type Property

n_objective_funs
number of objective functions

Returns Number of objective functions

Return type int

Type Property

name
name

Returns Name of the constraint

Return type str

Type Property

Methods Documentation

evaluate(*decision_vector*, *objective_vector*)
Evaluate the constraint.

This evaluates the constraint and return a float indicating how and if the constraint was violated. A negative value indicates a violation and a positive value indicates a non-violation.

Parameters

- **decision_vector** (*np.ndarray*) – A decision_vector containing the values of the decision variables.
- **objective_vector** (*np.ndarray*) – A decision_vector containing the values of the objective functions.

Returns A float indicating how the constraint holds.

Return type float

Raises ***ConstraintError*** – When something goes wrong evaluating the constraint or the objectives and decision vectors are of wrong shape.

ConstraintError

exception desdeo_problem.problem.**ConstraintError**
Raised when an error related to the Constraint class in encountered.

ConstraintBase

class desdeo_problem.problem.**ConstraintBase**
Bases: abc.ABC

Base class for constraints.

Methods Summary

evaluate(decision_vector, objective_vector)	Evaluate the constraint functions.

Methods Documentation

abstract evaluate(*decision_vector*, *objective_vector*)
Evaluate the constraint functions.

This function will evaluate constraints and return a float indicating how severely the constraint has been broken.

Parameters

- **decision_vector** (*np.ndarray*) – A decision_vector containing the decision variable values.
- **objective_vector** (*np.ndarray*) – A decision_vector containing the objective function values.

Returns A float representing how and if the constraint has been violated. A positive value represents no violation and a negative value represents a violation. The absolute value of the returned float functions as an indicator of the severity of the violation (or how well the constraint holds, if the returned value of positive).

Return type float

ObjectiveBase

class desdeo_problem.problem.**ObjectiveBase**
Bases: abc.ABC

The abstract base class for objectives.

Methods Summary

evaluate(decision_vector[, use_surrogate])	Evaluates the objective according to a decision variable vector.

Methods Documentation

evaluate (*decision_vector*, *use_surrogate=False*)
Evaluates the objective according to a decision variable vector.

Uses surrogate model if use_surrogates is true. If use_surrogates is False, uses func_evaluate which evaluates using the true objective function.

Parameters

- **decision_vector** (*np.ndarray*) – A vector of Variables to be used in the evaluation of the objective.
- **use_surrogate** (*bool*) – A boolean which determines whether to use surrogates or true function evaluator. False by default.

Return type ObjectiveEvaluationResults

ObjectiveError

exception desdeo_problem.problem.**ObjectiveError**
Raised when an error related to the Objective class is encountered.

ObjectiveEvaluationResults

class desdeo_problem.problem.**ObjectiveEvaluationResults**(*objectives: Union[float, numpy.ndarray]*, *uncertainity: Union[None, float, numpy.ndarray] = None*)

Bases: tuple

The return object of <problem>.evaluate methods.

objectives
The objective function value/s for the input vector.

Type Union[float, np.ndarray]

uncertainity
The uncertainity in the objective value/s.

Type Union[None, float, np.ndarray]

VectorObjectiveBase

class desdeo_problem.problem.**VectorObjectiveBase**
Bases: abc.ABC

The abstract base class for multiple objectives which are calculated at once.

Methods Summary

evaluate(decision_vector[, use_surrogate])	Evaluates the objective according to a decision variable vector.

Methods Documentation

evaluate(*decision_vector*, *use_surrogate=False*)
Evaluates the objective according to a decision variable vector.

Uses surrogate model if use_surrogates is true. If use_surrogates is False, uses func_evaluate which evaluates using the true objective function.

Parameters

- **decision_vector** (*np.ndarray*) – A vector of Variables to be used in the evaluation of the objective.
- **use_surrogate** (*bool*) – A boolean which determines whether to use surrogates or true function evaluator. False by default.

Return type ObjectiveEvaluationResults

ScalarObjective

class desdeo_problem.problem.**ScalarObjective**(*name*, *evaluator*, *lower_bound=- inf*, *upper_bound=inf*, *maximize=None*)
Bases: desdeo_problem.problem.Objective.ObjectiveBase

A simple objective function that returns a scalar.

To be depreciated

Parameters

- **name** (*str*) – Name of the objective.
- **evaluator** (*Callable*) – The function to evaluate the objective's value.
- **lower_bound** (*float*) – The lower bound of the objective.
- **upper_bound** (*float*) – The upper bound of the objective.
- **maximize** (*bool*) – Boolean to determine whether the objective is to be maximized.

__name
Name of the objective.

Type str

__value
The current value of the objective function.

Type float

__evaluator
The function to evaluate the objective's value.

Type Callable

__lower_bound
The lower bound of the objective.

Type float

__upper_bound
The upper bound of the objective.

Type float

maximize
List of boolean to determine whether the objectives are to be maximized. All false by default

Type List[bool]

Raises *ObjectiveError* – When ill formed bounds are given.

Attributes Summary

evaluator	evaluator for the objective
lower_bound	lower bound of the objective.
name	name
upper_bound	upper bound of the objective.
value	value

Attributes Documentation

evaluator
evaluator for the objective

Returns evaluator

Return type callable

Type Property

lower_bound
lower bound of the objective.

Returns lower bound of the objective

Return type float

Type Property

name
name

Returns name

Return type str

Type Property

upper_bound
upper bound of the objective.

Returns upper bound of the objective

Return type float

Type Property

value
value

Returns value

Return type float

Type Property

_ScalarObjective

class desdeo_problem.problem.**_ScalarObjective**(*name*, *evaluator*, *lower_bound=- inf*, *upper_bound=inf*, *maximize=None*)

Bases: desdeo_problem.problem.Objective.ScalarObjective

VectorObjective

class desdeo_problem.problem.**VectorObjective**(*name*, *evaluator*, *lower_bounds=None*, *upper_bounds=None*, *maximize=None*)

Bases: desdeo_problem.problem.Objective.VectorObjectiveBase

An objective object that calculated one or more objective functions.

To be renamed to Objective

Attributes: __name (List[str]): Names of the various objectives in a list __evaluator (Callable): The function that evaluates the objective values __lower_bounds (Union[List[float], np.ndarray), optional): Lower bounds

of the objective values. Defaults to None.

__upper_bounds (Union[List[float], np.ndarray), optional): Upper bounds of the objective values. Defaults to None.

__maximize (List[bool]): *List* of boolean to determine whether the objectives are to be maximized. All false by default

__n_of_objects (int): The number of objectives

Parameters

- **name** (*List[str]*) – Names of the various objectives in a list
- **evaluator** (*Callable*) – The function that evaluates the objective values
- **lower_bounds** (*Union[List[float], np.ndarray), optional*) – Lower bounds of the objective values. Defaults to None.
- **upper_bounds** (*Union[List[float], np.ndarray), optional*) – Upper bounds of the objective values. Defaults to None.

- **maximize** (Optional[List[bool]]) – *List* of boolean to determine whether the objectives are to be maximized. All false by default

Attributes Summary

evaluator	evaluator
lower_bounds	lower bounds
n_of_objectives	number of objectives
name	name
upper_bounds	upper bounds
values	values

Attributes Documentation

evaluator
evaluator

Returns Evaluator of the objective

Return type Callable

Type Property

lower_bounds
lower bounds

Returns lower bounds for vector valued objective.

Return type np.ndarray

Type Property

n_of_objectives
number of objectives

Returns the number of objectives

Return type int

Type Property

name
name

Returns name of the objective

Return type str

Type Property

upper_bounds
upper bounds

Returns upper bounds for vector valued objective.

Return type np.ndarray

Type Property

values
values

Returns Evaluated value and uncertainty of evaluation

Return type Tuple[float]

Type Property

ScalarDataObjective

class desdeo_problem.problem.**ScalarDataObjective**(*name*, *data*, *evaluator=None*, *lower_bound=-inf*, *upper_bound=inf*, *maximize=None*)

Bases: desdeo_problem.problem.Objective.ScalarObjective

A simple Objective class for single valued objectives.

To be depreciated.

Use when the an evaluator/simulator returns a single objective value or when there is no evaluator/simulator

X
Dataframe with corresponds the points where the objective value is known.

Type pd.DataFrame

y
The objective values corresponding the points.

Type pd.Series

variable_names
The names of the variables in X

Type pd.Index

_model
Model of the data

Type *BaseRegressor*

Parameters

- **name** (*List[str]*) – The name of the objective. Should be the same as a column name in the data.
- **data** (*pd.DataFrame*) – The data in a pandas dataframe. The columns should be named after variables/objective.
- **evaluator** (*Union[None, Callable], optional*) – A python function that contains the analytical function or calls the simulator to get the true objective value. By default None, as this is not required.
- **lower_bound** (*float, optional*) – Lower bound of the objective, by default -np.inf
- **upper_bound** (*float, optional*) – Upper bound of the objective, by default np.inf
- **maximize** (*List[bool], optional*) – Boolean describing whether the objective is to be maximized or not, by default None, which defaults to [False], hence minimizes.

Raises ***ObjectiveError*** – When the name provided during initialization does not match any name in the columns of the data provided during initilizaiton.

Methods Summary

train(model[, model_parameters, index, data])	Train surrogate model for the objective.

Methods Documentation

train (*model*, *model_parameters=None*, *index=None*, *data=None*)
Train surrogate model for the objective.

Parameters

- **model** (*BaseRegressor*) – A regressor. The regressor, when initialized, should have a fit method and a predict method. The predict method should return the predicted objective value, as well as the uncertainity value, in a tuple. If the regressor does not support calculating uncertainity, return a tuple of objective value and None.
- **model_parameters** (*Dict*) – **model_parameters is passed to the model when initialized.
- **index** (*List[int], optional*) – Indices of the samples (in self.X and self.y), to be used to train the surrogate model. By default None, which trains the model on the entire dataset. This behaviour may be changed in the future to support test-train split or cross validation.
- **data** (*pd.DataFrame, optional*) – Extra data to be used for training only. This data is not saved. By default None, which then uses self.X and self.y for training.

Raises ***ObjectiveError*** – For unexpected errors

_ScalarDataObjective

class desdeo_problem.problem.**_ScalarDataObjective**(*name*, *data*, *evaluator=None*, *lower_bound=-inf*, *upper_bound=inf*, *maximize=None*)
Bases: desdeo_problem.problem.Objective.ScalarDataObjective

VectorDataObjective

class desdeo_problem.problem.**VectorDataObjective**(*name*, *data*, *evaluator=None*, *lower_bounds=None*, *upper_bounds=None*, *maximize=None*)
Bases: desdeo_problem.problem.Objective.VectorObjective

A Objective class for multi/valued objectives.

Use when the an evaluator/simulator returns a multiple objective values or when there is no evaluator/simulator.

X
Dataframe with corresponds the points where the objective value is known.

Type pd.DataFrame

y
The objective values corresponding the points.

Type pd.Series

variable_names
The names of the variables in X

Type pd.Index

_model
BaseRegressor (or None if not trained) models for each objective, keys are the names of objectives.

Type Dict

_model_trained
boolean if model is trained for each objective, keys are the names of objectives. Default false.

Type Dict

Parameters

- **name** (*List[str]*) – The name of the objective. Should be the same as a column name in the data.
- **data** (*pd.DataFrame*) – The data in a pandas dataframe. The columns should be named after variables/objective.
- **evaluator** (*Union[None, Callable], optional*) – A python function that contains the analytical function or calls the simulator to get the true objective value. By default None, as this is not required.
- **lower_bound** (*float, optional*) – Lower bound of the objective, by default -np.inf
- **upper_bound** (*float, optional*) – Upper bound of the objective, by default np.inf
- **maximize** (*List[bool], optional*) – Boolean describing whether the objective is to be maximized or not, by default None, which defaults to [False], hence minimizes.

Raises ***ObjectiveError*** – When the name provided during initialization does not match any name in the columns of the data provided during initilizaiton.

Methods Summary

train(models[, model_parameters, index, data])	Train surrogate models for the objective.

Methods Documentation

train(*models*, *model_parameters=None*, *index=None*, *data=None*)
Train surrogate models for the objective.

Parameters

- **model** (*BaseRegressor or List[BaseRegressors]*) – A regressor or a list of regressors. The regressor/s, when initialized, should have a fit method and a predict method. The predict method should return the predicted objective value, as well as the uncertainity value, in a tuple. If the regressor does not support calculating uncertainity, return a tuple of objective value and None. If a single regressor is provided, that regressor is used for all the objectives. If a list of regressors is provided, and if the list contains one regressor for each objective, then those individual regressors are used to model the objectives. If the number of regressors is not equal to the number of objectives, an error is raised.

- **model_parameters** (*Dict or List[Dict]*) – The parameters for the regressors. Should be a dict if a single regressor is provided. If a list of regressors is provided, the parameters should be in a list of dicts, same length as the list of regressors(= number of objs).
- **index** (*List[int], optional*) – Indices of the samples (in self.X and self.y), to be used to train the surrogate model. By default None, which trains the model on the entire dataset. This behaviour may be changed in the future to support test-train split or cross validation.
- **data** (*pd.DataFrame, optional*) – Extra data to be used for training only. This data is not saved. By default None, which then uses self.X and self.y for training.

Raises

- ***ObjectiveError*** – If the formats of the model and model parameters do not match
- ***ObjectiveError*** – If the lengths of list of models and/or model parameter dictionaries are not equal to the number of objectives.

ProblemError

exception desdeo_problem.problem.**ProblemError**
Raised when an error related to the Problem class is encountered.

ProblemBase

class desdeo_problem.problem.**ProblemBase**
Bases: abc.ABC

The base class for the problems.

All other problem classes should be derived from this.

nadir
Nadir values for the problem, initiated = None

Type np.ndarray

ideal
Ideal values for the problem, initiated = None

Type np.ndarray

nadir_fitness
Fitness values for nadir, initiated = None

Type np.ndarray

ideal_fitness
Fitness values for ideal, initiated = None

Type np.ndarray

__n_of_objectives
Number of objectives, initiated = 0

Type int

__n_of_variables
Number of variables, initiated = 0

Type int

__decision_vectors
Array of decision variable vectors, initiated = None

Type np.ndarray

__objective_vectors
Array of objective variable vectors, initiated = None

Type np.ndarray

Attributes Summary

decision_vectors	Property, returns the decision variable vectors array.
n_of_objectives	Property, returns the number of objectives.
n_of_variables	Property, returns the number of variables.

Methods Summary

evaluate(decision_vectors[, use_surrogate])	Abstract method to evaluate problem.
evaluate_constraint_values()	Abstract method to evaluate constraint values.
get_variable_bounds()	Abstract method to get variable bounds

Attributes Documentation

decision_vectors
Property, returns the decision variable vectors array.

Returns decision vector array

Return type np.ndarray

n_of_objectives
Property, returns the number of objectives.

Returns The number of objectives

Return type int

n_of_variables
Property, returns the number of variables.

Returns The number of variables

Return type int

Methods Documentation

abstract evaluate(*decision_vectors*, *use_surrogate=False*)
Abstract method to evaluate problem.

Evaluates the problem using an ensemble of input vectors. Uses surrogate models if available. Otherwise, it uses the true evaluator.

Parameters

- **decision_vectors** (*np.ndarray*) – An array of decision variable
- **vectors.** (*input*) –
- **use_surrogate** (*bool*) – A bool to control whether to use the true, potentially
- **function or a surrogate model to evaluate the objectives.** (*expensive*) –

Returns

Dict with the following keys:

'objectives' (np.ndarray): The objective function values for each input vector.

'constraints' (Union[np.ndarray, None]): The constraint values of the problem corresponding each input vector.

'fitness' (np.ndarray): Equal to objective values if objective is to be minimized. Multiplied by (-1) if objective to be maximized.

'uncertainity' (Union[np.ndarray, None]): The uncertainity in the objective values.

Return type (Dict)

abstract evaluate_constraint_values()
Abstract method to evaluate constraint values.

Evaluate just the constraint function values using the attributes decision_vectors and objective_vectors

Note: Currently not supported by ScalarMOProblem

Return type Optional[ndarray]

abstract get_variable_bounds()
Abstract method to get variable bounds

Return type Optional[ndarray]

EvaluationResults

class desdeo_problem.problem.**EvaluationResults**(*objectives: numpy.ndarray*, *fitness: numpy.ndarray*, *constraints: Union[None, numpy.ndarray] = None*, *uncertainity: Union[None, numpy.ndarray] = None*)

Bases: tuple

The return object of <problem>.evaluate methods.

objectives
The objective function values for each input vector.

Type np.ndarray

fitness
Equal to objective values if objective is to be minimized. Multiplied by (-1) if objective to be maximized.

Type np.ndarray

constraints
The constraint values of the problem corresponding each input vector.

Type Union[None, np.ndarray]

uncertainity
The uncertainity in the objective values.

Type Union[None, np.ndarray]

ScalarMOProblem

class desdeo_problem.problem.**ScalarMOProblem**(*objectives*, *variables*, *constraints*, *nadir=None*, *ideal=None*)

Bases: desdeo_problem.problem.Problem.ProblemBase

A multiobjective optimization problem.

To be depreciated.

A multiobjective optimization problem with user defined objective functions, constraints and variables. The objectives each return a single scalar.

Parameters

- **objectives** (*List[ScalarObjective]*) – A list containing the objectives of the problem.
- **variables** (*List[Variable]*) – A list containing the variables of the problem.
- **constraints** (*List[ScalarConstraint]*) – A list containing the constraints of the problem. If no constraints exist, None may be supllied as the value.
- **nadir** (*Optional[np.ndarray]*) – The nadir point of the problem.
- **ideal** (*Optional[np.ndarray]*) – The ideal point of the problem.

__n_of_objectives
The number of objectives in the problem.

Type int

__n_of_variables
The number of variables in the problem.

Type int

__n_of_constraints
The number of constraints in the problem.

Type int

__nadir
The nadir point of the problem.

Type np.ndarray

__ideal
The ideal point of the problem.

Type np.ndarray

__objectives
A list containing the objectives of the problem.

Type List[*ScalarObjective*]

__constraints
A list conatining the constraints of the problem.

Type List[*ScalarConstraint*]

Raises ***ProblemError*** – Ill formed nadir and/or ideal vectors are supplied.

Attributes Summary

constraints	the list of constraints.
ideal	the ideal point of the problem.
n_of_constraints	the number of constraints.
n_of_objectives	the number of objectives.
n_of_variables	the number of variables.
nadir	the nadir point of the problem.
objectives	the list of objectives.
variables	the list of problem variables.

Methods Summary

evaluate(decision_vectors[, use_surrogate])	Evaluates the problem using an ensemble of input vectors.
evaluate_constraint_values()	Evaluate constraint values.
get_objective_names()	Get objective names.
get_uncertainty_names()	Return the names of the objectives present in the problem in the order they were added.
get_variable_bounds()	Get the variable bounds.
get_variable_lower_bounds()	Get variable lower bounds.
get_variable_names()	Get variable names.
get_variable_upper_bounds()	Get variable upper bounds.

Attributes Documentation

constraints
the list of constraints.

Returns the list of constraints

Return type List[*_ScalarObjective*]

Type Property

ideal: numpy.ndarray
the ideal point of the problem.

Returns the ideal point of the problem.

Return type np.ndarray

Type Property

n_of_constraints
the number of constraints.

Returns the number of constraints.

Return type int

Type Property

n_of_objectives
the number of objectives.

Returns the number of objectives.

Return type int

Type Property

n_of_variables
the number of variables.

Returns the number of variables.

Return type int

Type Property

nadir: numpy.ndarray
the nadir point of the problem.

Returns the nadir point of the problem.

Return type np.ndarray

Type Property

objectives
the list of objectives.

Returns the list of objectives

Return type List[*ScalarObjective*]

Type Property

variables
the list of problem variables.

Returns the list of problem variables

Return type List[*_ScalarObjective*]

Type Property

Methods Documentation

evaluate(*decision_vectors*, *use_surrogate=False*)
Evaluates the problem using an ensemble of input vectors.

Parameters **decision_vectors** (*np.ndarray*) – An 2D array of decision variable input vectors. Each column represent the values of each decision variable.

Returns

If constraint are defined, returns the objective vector values and corresponding constraint values. Or, if no constraints are defined, returns just the objective vector values with None as the constraint values.

Return type Tuple[np.ndarray, Union[None, np.ndarray]]

Raises ***ProblemError*** – The decision_vectors have wrong dimensions.

evaluate_constraint_values()
Evaluate constraint values.

Evaluate just the constraint function values using the attributes decision_vectors and objective_vectors

Raises **NotImplementedError** –

Note: Currently not supported by ScalarMOProblem

Return type Optional[ndarray]

get_objective_names()
Get objective names.

Return the names of the objectives present in the problem in the order they were added.

Returns Names of the objectives in the order they were added.

Return type List[str]

get_uncertainty_names()
Return the names of the objectives present in the problem in the order they were added.

Returns Names of the objectives in the order they were added.

Return type List[str]

get_variable_bounds()
Get the variable bounds.

Return the upper and lower bounds of each decision variable present in the problem as a 2D numpy array. The first column corresponds to the lower bounds of each variable, and the second column to the upper bound.

Returns Lower and upper bounds of each variable as a 2D numpy array. If undefined variables, return None instead.

Return type np.ndarray

get_variable_lower_bounds()
Get variable lower bounds.

Return the lower bounds of each variable as a list. The order of the bounds follows the order the variables were added to the problem.

Returns An array with the lower bounds of the variables.

Return type np.ndarray

get_variable_names()
Get variable names.

Return the variable names of the variables present in the problem in the order they were added.

Returns Names of the variables in the order they were added.

Return type List[str]

get_variable_upper_bounds()
Get variable upper bounds.

Return the upper bounds of each variable as a list. The order of the bounds follows the order the variables were added to the problem. :returns: An array with the upper bounds of the variables. :rtype: np.ndarray

ScalarDataProblem

class desdeo_problem.problem.**ScalarDataProblem**(*decision_vectors*, *objective_vectors*)
Bases: desdeo_problem.problem.Problem.ProblemBase

A problem class for case where the data is pre-computed.

To be depreciated

Defines a problem with pre-computed data representing a multiobjective optimization problem with scalar valued objective functions.

Parameters

- **decision_vectors** (*np.ndarray*) – A 2D vector of decision_vectors. Each row represents a solution with the value for each decision_vectors defined on the columns.
- **objective_vectors** (*np.ndarray*) – A 2D vector of objective function values. Each row represents one objective vector with the values for the invidual objective functions defined on the columns.

decision_vectors
See args

Type np.ndarray

objective_vectors
See args

Type np.ndarray

__epsilon
A small floating point number to shift the bounds of the variables. See, get_variable_bounds, default value 1e-6

Type float

__constraints
A list of defined constraints.

Type List[*ScalarConstraint*]

nadir
The nadir point of the problem.

Type np.ndarray

ideal
The ideal point of the problem.

Type np.ndarray

__model_exists
is there a model for this problem

Type bool

Note: It is assumed that the decision_vectors and objectives follow a direct one-to-one mapping, i.e., the objective values on the ith row in 'objectives' should represent the solution of the multiobjective problem when evaluated with the decision_vectors on the ith row in 'decision_vectors'.

Attributes Summary

constraints	Constraints.
epsilon	epsilon.

Methods Summary

evaluate(decision_vectors)	Evaluate the values of the objectives at the given decision.
evaluate_constraint_values()	Evaluate the constraint values.
get_variable_bounds()	Get the variable bounds.

Attributes Documentation

constraints
Constraints.

Returns list of the defined constraints

Return type List[*ScalarConstraint*]

Type Property

epsilon
epsilon.

Returns epsilon value (for shifting the bounds of variables)

Return type float

Type Property

Methods Documentation

evaluate(*decision_vectors*)
Evaluate the values of the objectives at the given decision.

Evaluate the values of the objectives corresponding to the decision decision_vectors.

Parameters **decision_vectors** (*np.ndarray*) – A 2D array with the decision decision_vectors to be evaluated on each row.

Returns

A 2D array with the objective values corresponding to each decision vectors on the rows.

Return type nd.ndarray

Note: At the moment, this function just maps the given decision decision_vectors to the closest decision variable present (using an L2 distance) in the problem and returns the corresponsing objective vector.

---

evaluate_constraint_values()
Evaluate the constraint values.

Evaluate the constraint values for each defined constraint. A positive value indicates that a constraint is adhered to, a negative value indicates a violated constraint.

Returns

A 2D array with each row representing the constraint values for different objective vectors. One column for each constraint. If no constraint function are defined, returns None.

Return type Optional[np.ndarray]

get_variable_bounds()
Get the variable bounds.

Returns

The variable bounds in a stack. The epsilon value will be added to the upper bounds and substracted from the lower bounds to return closed bounds.

Return type np.array[float]

Note: If self.epsilon is zero, the bounds will represent an open range.

MOProblem

class desdeo_problem.problem.**MOProblem**(*objectives*, *variables*, *constraints=None*, *nadir=None*, *ideal=None*)
Bases: desdeo_problem.problem.Problem.ProblemBase

An user defined multiobjective optimization problem.

A multiobjective optimization problem with user defined objective functions, constraints, and variables.

Parameters

- **objectives** (*List[Union[ScalarObjective, VectorObjective]]*) – A list containing the objectives of the problem.

- **variables** (*List[Variable]*) – A list containing the variables of the problem.
- **constraints** (*List[ScalarConstraint]*) – A list of the constraints of the problem.
- **nadir** (*Optional[np.ndarray], optional*) – Nadir point of the problem. Defaults to None.
- **ideal** (*Optional[np.ndarray], optional*) – Ideal point of the problem. Defaults to None.

__objectives
A list containing the objectives of the problem.

Type List[Union[*ScalarObjective*, *VectorObjective*]]

__variables
A list containing the variables of the problem.

Type List[*Variable*]

__constraints
A list of the constraints of the problem.

Type List[*ScalarConstraint*]

__nadir
Nadir point of the problem. Defaults to None.

Type Optional[np.ndarray], optional

__ideal
Ideal point of the problem. Defaults to None.

Type Optional[np.ndarray], optional

__n_of_variables
The number of variables

Type int

__n_of_objectives
The number of objectives

Type int

Raises ***ProblemError*** – If ideal or nadir vectors are not the same size as number of objectives.

Attributes Summary

constraints	list of constraints.
n_of_constraints	number of constraints.
n_of_objectives	number of objectives.
n_of_variables	number of variables.
objectives	list of objectives.
variables	List of variables

Methods Summary

evaluate(decision_vectors[, use_surrogate])	Evaluates the problem using an ensemble of input vectors.
evaluate_constraint_values(decision_vectors, ...)	Evaluate constraint values
evaluate_fitness(objective_vectors)	Evaluate fitness of the objectives.
evaluate_objectives(decision_vectors[, ...])	Evaluate objective values of the problem
get_objective_names()	Get objective names.
get_variable_bounds()	Get variable bounds.
get_variable_lower_bounds()	Get variable lower bounds.
get_variable_names()	Get variable names.
get_variable_upper_bounds()	Get variable upper bounds.
number_of_objectives(obj_instance)	Return the number of objectives in the given obj_instance.
update_ideal(objective_vectors, fitness)	Update the ideal vector

Attributes Documentation

constraints
list of constraints.

Returns list of constraints

Return type List[*ScalarConstraint*]

Type Property

n_of_constraints
number of constraints.

Returns Number of constraints

Return type int

Type Property

n_of_objectives
number of objectives.

Returns number of objectives

Return type int

Type Property

n_of_variables
number of variables.

Returns Number of variables.

Return type int

Type Property

objectives
list of objectives.

Returns list of objectives

Return type List[*ScalarObjective*]

Type Property

variables
List of variables

Returns list of variables

Return type List[*Variable*]

Type Property

Methods Documentation

evaluate(*decision_vectors*, *use_surrogate=False*)
Evaluates the problem using an ensemble of input vectors.

Parameters

- **decision_vectors** (*np.ndarray*) – An 2D array of decision variable input vectors. Each column represent the values of each decision variable.
- **use_surrogate** (*bool*) – A bool to control whether to use the true, potentially expensive function or a surrogate model to evaluate the objectives.

Returns If constraint are defined, returns the objective vector values and corresponding constraint values. Or, if no constraints are defined, returns just the objective vector values with None as the constraint values.

Return type Tuple[np.ndarray, Union[None, np.ndarray]]

Raises

- ***ProblemError*** – The decision_vectors have wrong dimensions.
- **ValueError** – If decision_vectors violate the lower or upper bounds.

evaluate_constraint_values(*decision_vectors*, *objective_vectors*)
Evaluate constraint values

Evaluate just the constraint function values using the attributes decision_vectors and objective_vectors

Parameters

- **decision_vectors** (*np.ndarray*) – An 2D array of decision variable input vectors. Each column represent the values of each decision variable.
- **use_surrogate** (*bool*) – A bool to control whether to use the true, potentially expensive function or a surrogate model to evaluate the objectives.

Returns

if there are constraints, then this returns np.ndarray of constraint values, else returns None

Return type Optional[np.ndarray]

Raises **NotImplementedError** –

Note: Currently not supported by ScalarMOProblem

evaluate_fitness(*objective_vectors*)
Evaluate fitness of the objectives.

Parameters **objective_vectors** (*np.ndarray*) – objective vector array

Returns fitness of each objective vector

Return type np.ndarray

evaluate_objectives(*decision_vectors*, *use_surrogate=False*)
Evaluate objective values of the problem

Parameters

- **decision_vectors** (*np.ndarray*) – An 2D array of decision variable input vectors. Each column represent the values of each decision variable.
- **use_surrogate** (*bool*) – A bool to control whether to use the true, potentially expensive function or a surrogate model to evaluate the objectives.

Returns Objective vector values with their uncertainty.

Return type Tuple[np.ndarray]

get_objective_names()
Get objective names. Return the names of the objectives present in the problem in the order they were added.

Returns Names of the objectives in the order they were added.

Return type List[str]

get_variable_bounds()
Get variable bounds. Return the upper and lower bounds of each decision variable present in the problem as a 2D numpy array. The first column corresponds to the lower bounds of each variable, and the second column to the upper bound.

Returns Lower and upper bounds of each variable as a 2D numpy array. If undefined variables, return None instead.

Return type np.ndarray

get_variable_lower_bounds()
Get variable lower bounds.

Return the lower bounds of each variable as a list. The order of the bounds follows the order the variables were added to the problem.

Returns An array with the lower bounds of the variables.

Return type np.ndarray

get_variable_names()
Get variable names. Return the variable names of the variables present in the problem in the order they were added.

Returns Names of the variables in the order they were added.

Return type List[str]

get_variable_upper_bounds()
Get variable upper bounds.

Return the upper bounds of each variable as a list. The order of the bounds follows the order the variables were added to the problem.

Returns An array with the upper bounds of the variables.

Return type np.ndarray

static number_of_objectives(*obj_instance*)
Return the number of objectives in the given obj_instance.

Parameters **obj_instance** (*Union[ScalarObjective, VectorObjective]*) – An instance of one of the objective classes

Raises ***ProblemError*** – Raised when obj_instance is not an instance of the supported classes

Returns Number of objectives in obj_instance

Return type int

update_ideal(*objective_vectors*, *fitness*)
Update the ideal vector

Parameters

- **objective_vectors** (*np.ndarray*) – Objective vectors
- **fitness** (*np.ndarray*) – fittness of objective vectors.

DataProblem

class desdeo_problem.problem.**DataProblem**(*data*, *variable_names*, *objective_names*, *bounds=None*, *maximize=None*, *objectives=None*, *variables=None*, *constraints=None*, *nadir=None*, *ideal=None*)
Bases: desdeo_problem.problem.Problem.MOProblem

A class for a data based problem.

A problem class for data-based problem. This supports surrogate modelling. Data should be given in the form of a pandas dataframe.

Parameters

- **data** (*pd.DataFrame*) – The input data. This will be used for training the model.
- **variable_names** (*List[str]*) – Names of the variables in the dataframe provided.
- **objective_names** (*List[str]*) – Names of the objectices in the dataframe provided.
- **bounds** (*pd.DataFrame, optional*) – A pandas DataFrame containing the upper and lower bounds of the decision variables. Column names have to be same as variable_names. Row names have to be "lower_bound" and "upper_bound".
- **objectives** (*List[Union[ScalarDataObjective, VectorDataObjective,]], optional*) – Objective instances, currently not supported. Defaults to None.
- **variables** (*List[Variable], optional*) – Variable instances. Defaults to None. Currently not supported.
- **constraints** (*List[ScalarConstraint], optional*) – Constraint instances. Defaults to None, which means that there are no constraints.
- **nadir** (*Optional[np.ndarray], optional*) – Nadir of the problem. Defaults to None.

- **ideal** (*Optional[np.ndarray], optional*) – Ideal of the problem. Defaults to None.

Raises

- ***ProblemError*** – When input data is not a dataframe.
- ***ProblemError*** – When given objective or variable names are not in dataframe column
- **NotImplementedError** – When objective instances are passed
- **NotImplementedError** – When variable instances are passed

Methods Summary

train(models[, model_parameters, index, data])	Train surrogate models for all the objectives.
train_one_objective(name, model, ...[, ...])	Train one objective at a time, otherwise same is the train method.

Methods Documentation

train (*models*, *model_parameters=None*, *index=None*, *data=None*)
Train surrogate models for all the objectives.

The models should have a fit method and a predict method. The predict method should return predicted values as well as uncertainity value (even if they are none.)

Parameters

- **models** (*Union[BaseRegressor, List[BaseRegressor]]*) – The class for the surrogate modelling algorithm.
- **models_parameters** – Dict or List[Dict] The parameters for the regressors. Should be a dict if a single regressor is provided. If a list of regressors is provided, the parameters should be in a list of dicts, same length as the list of regressors(= number of objs).
- **index** (*List[int], optional*) – The indices of the samples to be used for training the surrogate model. If no values are proveded, all samples are used.
- **data** (*pd.DataFrame, optional*) – Use this argument if some external data is to be used for training. Defaults to None.

Raises

- ***ProblemError*** – If VectorDataObjective is used as one of the objective
- **instances. They are not supported yet.** –

train_one_objective (*name*, *model*, *model_parameters*, *index=None*, *data=None*)
Train one objective at a time, otherwise same is the train method.

Parameters

- **name** (*str*) – Name of the objective to be trained.
- **model** (*BaseRegressor*) – The class for the surrogate modelling algorithm.
- **model_parameters** (*Dict*) – **model_parameters is passed to the model when initialized.

- **index** (*List[int], optional*) – The indices of the samples to be used for training the surrogate model. If no values are proveded, all samples are used.
- **data** (*pd.DataFrame, optional*) – Use this argument if some external data is to be used for training. Defaults to None.

Raises

- ***ProblemError*** – If name is not in the list of objective names.
- ***ProblemError*** – If VectorDataObjective is used as one of the objective instances. They are not supported yet.

ExperimentalProblem

class desdeo_problem.problem.**ExperimentalProblem**(*variable_names*, *objective_names*, *uncertainity_names*, *evaluators=None*, *dimensions_data=None*, *data=None*, *objective_functions=None*, *constraints=None*)

Bases: desdeo_problem.problem.Problem.MOProblem

A problem class for data-based problem. This supports surrogate modelling. Data should be given in the form of a pandas dataframe. self.archive is created to save the true function evaluations and update the surrogate models if needed. self.archive updates whenever a true function evaluation happens.

Parameters

- **data** (*pd.DataFrame*) – The input data. This will be used for training the model.
- **variable_names** (*List[str]*) – Names of the variables in the dataframe provided.
- **objective_names** (*List[str]*) – Names of the objectices in the dataframe provided.
- **objectives** (*List[Union[ScalarDataObjective, VectorDataObjective,]], optional*) – Objective instances, currently not supported. Defaults to None.
- **variables** (*List[Variable], optional*) – Variable instances. Defaults to None. Currently not supported.
- **constraints** (*List[ScalarConstraint], optional*) – Constraint instances. Defaults to None, which means that there are no constraints.
- **nadir** (*Optional[np.ndarray], optional*) – Nadir of the problem. Defaults to None.
- **ideal** (*Optional[np.ndarray], optional*) – Ideal of the problem. Defaults to None.

Raises

- ***ProblemError*** – When input data is not a dataframe.
- ***ProblemError*** – When given objective or variable names are not in dataframe column
- **NotImplementedError** – When objective instances are passed
- **NotImplementedError** – When variable instances are passed

Note: not properly implemented!

Methods Summary

evaluate(decision_vectors, use_surrogate)	Evaluates the problem using an ensemble of input vectors.
train(models[, model_parameters, index, data])	Train surrogate models for all the objectives.
train_one_objective(name, model, ...[, ...])	Train one objective at a time, otherwise same is the train method.

Methods Documentation

evaluate(*decision_vectors*, *use_surrogate*)

Evaluates the problem using an ensemble of input vectors.

Parameters

- **decision_vectors** (*np.ndarray*) – An 2D array of decision variable input vectors. Each column represent the values of each decision variable.
- **use_surrogate** (*bool*) – A bool to control whether to use the true, potentially expensive function or a surrogate model to evaluate the objectives.

Returns If constraint are defined, returns the objective vector values and corresponding constraint values. Or, if no constraints are defined, returns just the objective vector values with None as the constraint values.

Return type Tuple[np.ndarray, Union[None, np.ndarray]]

Raises

- ***ProblemError*** – The decision_vectors have wrong dimensions.
- **ValueError** – If decision_vectors violate the lower or upper bounds.

train(*models*, *model_parameters=None*, *index=None*, *data=None*)

Train surrogate models for all the objectives.

The models should have a fit method and a predict method. The predict method should return predicted values as well as uncertainity value (even if they are none.)

Parameters

- **models** (*Union[BaseRegressor, List[BaseRegressor]]*) – The class for the surrogate modelling algorithm.
- **models_parameters** – Dict or List[Dict] The parameters for the regressors. Should be a dict if a single regressor is provided. If a list of regressors is provided, the parameters should be in a list of dicts, same length as the list of regressors(= number of objs).
- **index** (*List[int], optional*) – The indices of the samples to be used for training the surrogate model. If no values are proveded, all samples are used.
- **data** (*pd.DataFrame, optional*) – Use this argument if some external data is to be used for training. Defaults to None.

Raises ***ProblemError*** – If VectorDataObjective is used as one of the objective instances. They are not supported yet.

train_one_objective(*name*, *model*, *model_parameters*, *index=None*, *data=None*)
Train one objective at a time, otherwise same is the train method.

Parameters

- **name** (*str*) – Name of the objective to be trained.
- **model** (BaseRegressor) – The class for the surrogate modelling algorithm.
- **model_parameters** (*Dict*) – **model_parameters is passed to the model when initialized.
- **index** (*List[int], optional*) – The indices of the samples to be used for training the surrogate model. If no values are proveded, all samples are used.
- **data** (*pd.DataFrame, optional*) – Use this argument if some external data is to be used for training. Defaults to None.

Raises

- ***ProblemError*** – If name is not in the list of objective names.
- ***ProblemError*** – If VectorDataObjective is used as one of the objective instances. They are not supported yet.

VariableError

exception desdeo_problem.problem.**VariableError**
Raised when an error is encountered during the handling of the Variable objects.

VariableBuilderError

exception desdeo_problem.problem.**VariableBuilderError**
Raised when an error is encountered during the handling of the Variable objects.

Variable

class desdeo_problem.problem.**Variable**(*name*, *initial_value*, *lower_bound=-inf*, *upper_bound=inf*)
Bases: object

Simple variable with a name, initial value and bounds.

Parameters

- **name** (*str*) – Name of the variable
- **initial_value** (*float*) – The initial value of the variable.
- **lower_bound** (*float, optional*) – Lower bound of the variable. Defaults to negative infinity.
- **upper_bound** (*float, optional*) – Upper bound of the variable. Defaults to positive infinity.

name
Name of the variable.

Type str

initial_value
Initial value of the variable.

Type float

lower_bound
Lower bound of the variable.

Type float

upper_bound
Upper bound of the variable.

Type float

current_value
The current value the variable holds.

Type float

Raises *VariableError* – Bounds are incorrect.

Attributes Summary

current_value	current_value
initial_value	initial_value
name	name

Methods Summary

get_bounds()	Return the bounds of the variables as a tuple.

Attributes Documentation

current_value
current_value

Returns The current value of the variable

Return type float

Type Property

initial_value
initial_value

Returns The initial value of the variable.

Return type float

Type Property

name
name

Returns The name of the variable.

Return type str

Type Property

Methods Documentation

get_bounds()
Return the bounds of the variables as a tuple.

Returns

A tuple consisting of (lower_bound, upper_bound)

Return type tuple(float, float)

DiscreteDataProblem

class desdeo_problem.problem.**DiscreteDataProblem**(*data*, *variable_names*, *objective_names*, *ideal*, *nadir*)

Bases: object

A problem class for data-based problems with discrete values.

These data values are computed representing a set of non-dominated points.

Parameters

- **data** (*pd.DataFrame*) – The input data.
- **variable_names** (*List[str]*) – Names of the variables in the dataframe provided.
- **objective_names** (*List[str]*) – Names of the objectices in the dataframe provided.
- **nadir** (*np.ndarray*) – Nadir of the problem.
- **ideal** (*np.ndarray*) – Ideal of the problem.

Methods Summary

find_closest(x)	Find closest point in data to x.

Methods Documentation

find_closest(*x*)
Find closest point in data to x.

Given a vector of decision variables, finds the closest point in the given data and returns its index. A simple euclidean distance is used.

Parameters **x** (*np.ndarray*) – A 1D vector containing decision variables.

Returns The index of the closest point in the data computed for x.

Return type int

classificationPISProblem

class desdeo_problem.problem.**classificationPISProblem**(*objectives*, *variables*, *nadir*, *ideal*, *PIS*, *constraints=None*)

Bases: desdeo_problem.problem.Problem.MOProblem

A problem class for the IOPIS formulation for interactive optimization.

This variant uses the classification kind of preference information for the creation of the Preference incorporated space (PIS).

Parameters

- **objectives** (*List[Union[ScalarObjective, VectorObjective]]*) – A list containing the objectives of the problem.
- **variables** (*List[Variable]*) – A list containing the variables of the problem.
- **nadir** (*np.ndarray*) – Nadir point of the problem.
- **ideal** (*np.ndarray*) – Ideal point of the problem.
- **PIS** – An instantiated classificationPIS class from desdeo-tools.
- **constraints** (*List[ScalarConstraint], optional*) – A list of the constraints of the problem. Defaults to None.

Methods Summary

evaluate_fitness(objective_vectors)	Evaluate objective fitness.
reevaluate_fitness(objective_vectors)	Re-evaluate objective fitness.
update_ideal(objective_vectors, fitness)	Update ideal vector.
update_preference(preference)	Update PIS preference

Methods Documentation

evaluate_fitness(*objective_vectors*)

Evaluate objective fitness.

Parameters **objective_vectors** (*np.ndarray*) – objective vectors

Returns Objective fitness

Return type np.ndarray

reevaluate_fitness(*objective_vectors*)

Re-evaluate objective fitness.

Calls update_ideal with objective_vectors.

Parameters **objective_vectors** (*np.ndarray*) – objective vectors

Returns Objective fitness

Return type np.ndarray

update_ideal(*objective_vectors*, *fitness*)

Update ideal vector.

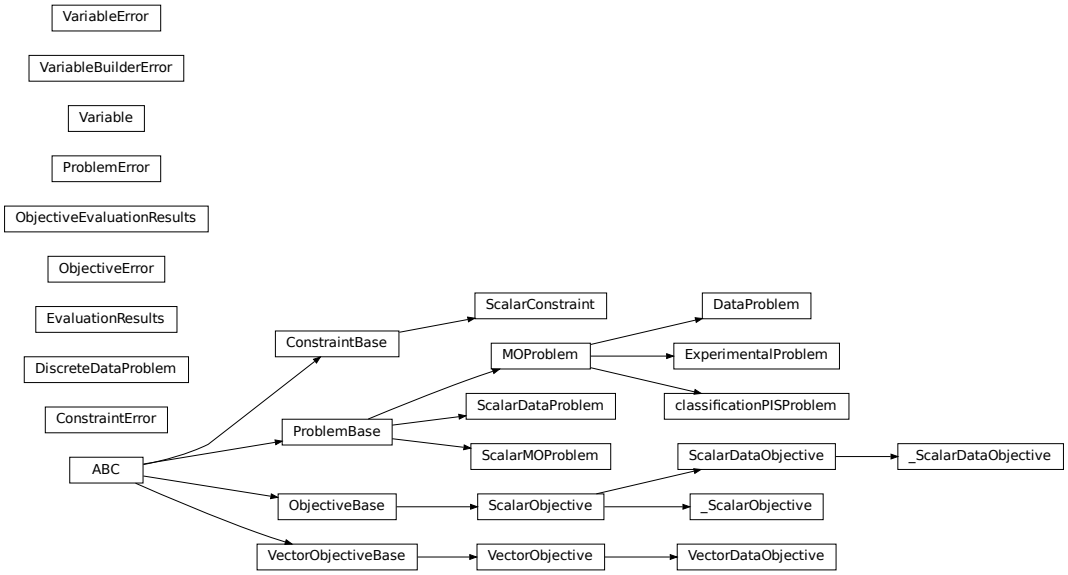
Parameters

- **objective_vectors** (*np.ndarray*) – Objective vectors
- **fitness** (*np.ndarray*) – Fitness values for objective vectors

update_preference(*preference*)
Update PIS preference

Parameters **preference** (*Dict*) – PIS preferences

Class Inheritance Diagram



desdeo_problem.testproblems Package

Functions

test_problem_builder(name[, n_of_variables, ...])	Build test problems.

test_problem_builder

desdeo_problem.testproblems.**test_problem_builder**(*name*, *n_of_variables=None*, *n_of_objectives=None*)

Build test problems. Currently supported: ZDT1-4, ZDT6, and DTLZ1-7.

Parameters

- **name** (*str*) – Name of the problem in all caps. For example: "ZDT1", "DTLZ4", etc.
- **n_of_variables** (*int, optional*) – Number of variables. Required for DTLZ problems, but can be skipped for ZDT problems as they only support one variable value.
- **n_of_objectives** (*int, optional*) – Required for DTLZ problems, but can be skipped for ZDT problems as they only support one variable value.

Raises ***ProblemError*** – When one of many issues occur while building the MOProblem instance.

Returns The test problem object

Return type *MOProblem*

desdeo_problem.surrogatemodels Package

Classes

ModelError	Raised when an error related to the surrogate models classes is encountered.
BaseRegressor()	
GaussianProcessRegressor(**kwargs)	
LipschitzianRegressor([L])	

ModelError

exception desdeo_problem.surrogatemodels.**ModelError**

Raised when an error related to the surrogate models classes is encountered.

BaseRegressor

class desdeo_problem.surrogatemodels.**BaseRegressor**
Bases: abc.ABC

Methods Summary

fit(X, y)	
predict(X)	**rtype** Tuple[ndarray, ndarray]

Methods Documentation

abstract fit(*X*, *y*)

abstract predict(*X*)

Return type Tuple[ndarray, ndarray]

GaussianProcessRegressor

class desdeo_problem.surrogatemodels.**GaussianProcessRegressor**(***kwargs*)
Bases: sklearn.gaussian_process._gpr.GaussianProcessRegressor, desdeo_problem.surrogatemodels.SurrogateModels.BaseRegressor

Methods Summary

predict(X)	Predict using the Gaussian process regression model

Methods Documentation

predict(*X*)
Predict using the Gaussian process regression model

We can also predict based on an unfitted model by using the GP prior. In addition to the mean of the predictive distribution, also its standard deviation (return_std=True) or covariance (return_cov=True). Note that at most one of the two can be requested.

Parameters

- **X** (*array-like of shape (n_samples, n_features) or list of object*) – Query points where the GP is evaluated.
- **return_std** (*bool, default=False*) – If True, the standard-deviation of the predictive distribution at the query points is returned along with the mean.
- **return_cov** (*bool, default=False*) – If True, the covariance of the joint predictive distribution at the query points is returned along with the mean.

Returns

- **y_mean** (*ndarray of shape (n_samples, [n_output_dims])*) – Mean of predictive distribution a query points.
- **y_std** (*ndarray of shape (n_samples,), optional*) – Standard deviation of predictive distribution at query points. Only returned when *return_std* is True.
- **y_cov** (*ndarray of shape (n_samples, n_samples), optional*) – Covariance of joint predictive distribution a query points. Only returned when *return_cov* is True.

LipschitzianRegressor

class desdeo_problem.surrogatemodels.**LipschitzianRegressor**(*L=None*)

Bases: desdeo_problem.surrogatemodels.SurrogateModels.BaseRegressor

Methods Summary

distance(array1, array2)
fit(X, y)
predict(X)
self_distance(arr)

Methods Documentation

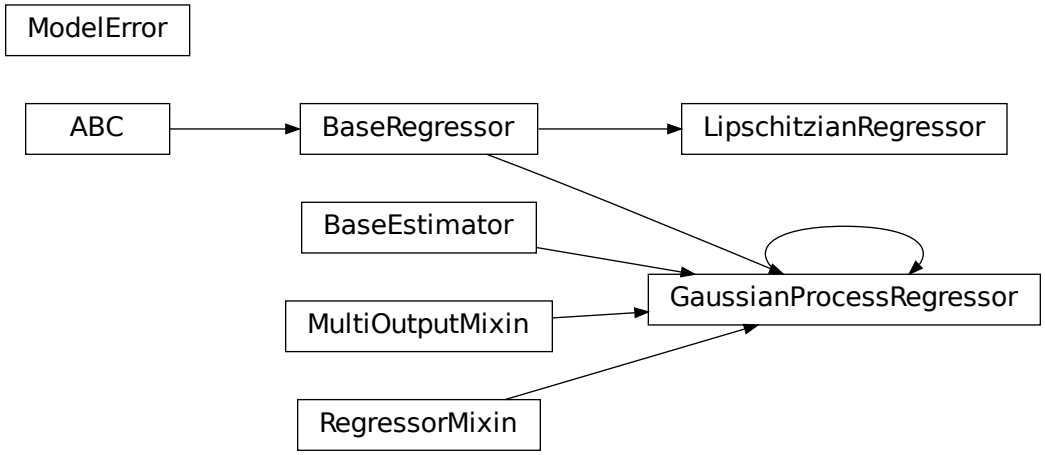
distance(*array1*, *array2*)

fit(*X*, *y*)

predict(*X*)

self_distance(*arr*)

Class Inheritance Diagram



2.2.2 Examples

Analytical problem

Defining a problem with an explicit mathematical representation is straightforward.

As an example, consider the following multiobjective optimization problem:

$$\begin{aligned} \min_{\mathbf{x}} \quad & x_1^2 - x_2; x_2^2 - 3x_1 \\ \text{s.t.} \quad & x_1 + x_2 \leq 10 \\ & \mathbf{x} \in S, \end{aligned} \tag{2.1}$$

where the feasible region is

$$x_i \in [-5, 5] \ \forall i \ \in [1, 2]\,. \tag{2.2}$$

Begin by importing the necessary classes:

[1]:
```
from desdeo_problem import Variable, ScalarObjective, ScalarConstraint,␣
↪ScalarMOProblem
```

Define the variables:

[2]:
```
# Args: name, starting value, lower bound, upper bound
x1 = Variable("x_1", 0, -0.5, 0.5)
x2 = Variable("x_2", 0, -0.5, 0.5)
```

Define the objectives, notice the argument of the callable objective function, it is assumed to be array-like.

[3]:
```
# Args: name, callable
obj1 = ScalarObjective("f_1", lambda x: x[:,0]**2 - x[:,1])
obj2 = ScalarObjective("f_2", lambda x: x[:,1]**2 - 3*x[:,0])
```

Define the constraints. Constraint may depend on objective function as well (second argument to the lambda, notice the underscore). In that case, the objectives should not be defined inline, like above, but as their own function definitions. The constraint should be defined so, that when evaluated, it should return a positive value, if the constraint is adhered to, and a negative, if the constraint is breached.

[4]:
```
# Args: name, n of variables, n of objectives, callable
cons1 = ScalarConstraint("c_1", 2, 2, lambda x, _: 10 - (x[:,0] + x[:,1]))
```

Finally, put it all together and create the problem.

[5]:
```
# Args: list of objevtives, variables and constraints
problem = ScalarMOProblem([obj1, obj2]
                          ,[x1, x2]
                          ,[cons1])
```

Now, the problem is fully specified and can be evaluated and played around with.

[6]:
```
import numpy as np

print("N of objectives:", problem.n_of_objectives)
print("N of variables:", problem.n_of_variables)
print("N of constraints:", problem.n_of_constraints)

res1 = problem.evaluate(np.array([2, 4]))
res2 = problem.evaluate(np.array([6, 6]))
res3 = problem.evaluate(np.array([[6, 3], [4,3], [7,4]]))

print("Single feasible decision variables:", res1.objectives, "with constraint values
↪", res1.constraints)
print("Single non-feasible decision variables:", res2.objectives, "with constraint␣
↪values", res2.constraints)
print("Multiple decision variables:", res3.objectives, "with constraint values", res3.
↪constraints)
```

```
N of objectives: 2
N of variables: 2
N of constraints: 1
Single feasible decision variables: [[ 0. 10.]] with constraint values [[4.]]
Single non-feasible decision variables: [[30. 18.]] with constraint values [[-2.]]
Multiple decision variables: [[33. -9.]
 [13. -3.]
 [45. -5.]] with constraint values [[ 1.]
 [ 3.]
 [-1.]]
```

[ ]:

The `Problem` class

An analytical problem is a problem where the mathematical formulation of the various objectives is known, as opposed to a data-driven problem, where one may need to train surrogate models to proceed with optimization.

The `Problem` class is the way to define optimization problems in the DESDEO framework. Once defined, the same `Problem` class instance can be used to solve optimization problems using various EAs from the `desdeo-emo` package, or the more traditional methods from the `desdeo-mcdm` package.

This notebook will help you understand how to instantiate a analytical problem object from scratch. The notebook will also go over other abstractions, namely classes for defining the decision variables, objectives, and the constraints, and will go over the functionalities provided by the abstractions.

Multiobjective Optimization Problem

Let's say that we have the following minimization problem:

$$
\begin{aligned}
\min_{\mathbf{x}} \quad & y_1, y_2, y_3 \\
& y_1 = x_1 + x_2 + x_3 \\
& y_2 = x_1 * x_2 * x_3 \\
& y_3 = x_1 * x_2 + x_3 \\
\text{s.t.} \quad & -2 \leq x_1 \leq 5 \\
& -1 \leq x_2 \leq 10 \\
& -0 \leq x_3 \leq 3 \\
& x_1 + x_2 + x_3 \leq 10 \\
& \mathbf{x} \in S,
\end{aligned}
\tag{2.3}
$$

Variables

Before instantiating the problem instance, we have to create object to define each of the variables, objectives, and constraints.

The variable objects can be created with the `desdeo_problem.Variable.Variable` class. This object stores the information related to the variable (such as, lower bound, upper bound, and an initial value). This information is used by the methods whenever required (such as when setting box constraints on searching algorithms or recombination operators) and for displaying results to the decision maker. Use this class to create variable objects, one variable at a time.

To define multiple `Variable` instances easily, use the `desdeo_problem.Variable.variable_builder` function. The function takes in all the necessary information for all the variables at once, and returns a List of `Variable` instances, one for each decision variable.

Use the `help()` function to know more about any function/class in the desdeo framework.

[1]:
```
from desdeo_problem import variable_builder

help(variable_builder)
```

```
Help on function variable_builder in module desdeo_problem.problem.Variable:

variable_builder(names: List[str], initial_values: Union[List[float], numpy.ndarray],␣
↪lower_bounds: Union[List[float], numpy.ndarray] = None, upper_bounds:␣
↪Union[List[float], numpy.ndarray] = None) -> List[desdeo_problem.problem.Variable.
↪Variable]
```

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```
    Automatically build all variable objects.

    Args:
        names (List[str]): Names of the variables
        initial_values (np.ndarray): Initial values taken by the variables.
        lower_bounds (Union[List[float], np.ndarray], optional): Lower bounds of the
            variables. If None, it defaults to negative infinity. Defaults to None.
        upper_bounds (Union[List[float], np.ndarray], optional): Upper bounds of the
            variables. If None, it defaults to positive infinity. Defaults to None.

    Raises:
        VariableError: Lengths of the input arrays are different.

    Returns:
        List[Variable]: List of variable objects
```

Let's build the `Variable` objects

[2]:
```
var_names = ["a", "b", "c"]  #  Make sure that the variable names are meaningful to␣
↪you.

initial_values = [1, 1, 1]
lower_bounds = [-2, -1, 0]
upper_bounds = [5, 10, 3]

variables = variable_builder(var_names, initial_values, lower_bounds, upper_bounds)
```

[3]:
```
print("Type of \"variables\": ", type(variables))
print("Length of \"variables\": ", len(variables))
print("Type of the contents of \"variables\": ", type(variables[0]))
```

```
Type of "variables":  <class 'list'>
Length of "variables":  3
Type of the contents of "variables":  <class 'desdeo_problem.problem.Variable.Variable
↪'>
```

Objectives

Objectives are defined using tha various objective classes found within the module `desdeo_problem.Objective`. To define an objective class instance, one needs to pass the following:

1. Objective name/s (Required): Name of the objective (or list of names, for multiple objective). This information will be used when displaying results to the user. Hence, these names must be understandable to the user.
2. Evaluator (Required for analytical/simulation based objectives): An evaluator is a python `Callable` which takes in the decision variables as it's input and returns the corresponding objective values. This python function can be used to connect to simulators outside the DESDEO framework.
3. Lower bound (Not required): A lower bound for the objective. This information can be used to generate approximate ideal/nadir point during optimization.
4. Upper bound (Not required): An upper bound for the objective. This information can be used to generate approximate ideal/nadir point during optimization.
5. maximize (Not required): This is a boolean value that determines whether an objective is to be maximized or minimized. This is `False` by default (i.e. the objective is minimized).

The DESDEO framework has the following classification for objectives, based on the kind of evaluater to be used:

1. "Scalar" objectives: If an evaluator/simulator evaluates only one objective, the objective is defined as a Scalar objective. Use the `desdeo_problem.Objective._ScalarObjective` class to handle such cases.
2. "Vector" objectives: If an evaluator evaluates and returns more than one objective at once, the set of objectives is defined as Vector objective. Use the `desdeo_problem.Objective.VectorObjective` class to handle such cases.

Note:`_ScalarObjective` will be depreciated in the future, and all of it's functionality will be handled by the `VectorObjective` class, which will be renamed to, simply, `Objective`.

To define a problem instance, the objectives may be defined as all Scalar objectives, all Vector objectives, or a mix of both, depending upon the case.

Let's see how to define and use both kinds of Objective classes:

[4]:
```
from desdeo_problem import ScalarObjective, VectorObjective

import numpy as np
```

Define the evaluators for the objectives. These evaluators should be python functions that take in the decision variable values and give out the objective value/s. The arguments of these evaluators are **2-D Numpy arrays**.

[5]:
```
def obj1_2(x):  #  This is a "simulator" that returns more than one objective at a␣
↪time. Hence, use VectorObjective
    y1 = x[:, 0] + x[:, 1] + x[:, 2]
    y2 = x[:, 0] * x[:, 1] * x[:, 2]
    return (y1, y2)


def obj3(x):  #  This is a "simulator" that returns only one objective at a time.␣
↪Hence, use ScalarObjective
    y3 = x[:, 0] * x[:, 1] + x[:, 2]
    return y3
```

Define the objectives. For this, you need the names of the objectives, and the evaluators defined above. If an evaluator returns multiple objective values, use the `VectorObjective` class to define those objectives. If an evaluator returns objective values for only one objective, either `VectorObjective` or `ScalarObjective` can be used.

If using `VectorObjective`, names should be provided in a list.

Additionaly, bounds of the objective values can also be provided.

[6]:
```
f1_2 = VectorObjective(["y1", "y2"], obj1_2)
f3 = ScalarObjective("y3", obj3, maximize=True)  # Note: f3 = VectorObjective(["y3"],␣
↪obj3) will also work.
```

Constraints

Constraint may depend on the decision variable values, as well as the objective function.

The constraint should be defined so, that when evaluated, it should return a positive value, if the constraint is adhered to, and a negative, if the constraint is breached.

[7]:
```
from desdeo_problem import ScalarConstraint

const_func = lambda x, y: 10 - (x[:, 0] + x[:, 1] + x[:, 2])
```

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```
# Args: name, number of variables, number of objectives, callable

cons1 = ScalarConstraint("c_1", 3, 3, const_func)
```

Creating the Problem object

Now that we have all the building blocks, we can create the problem object, using the `desdeo_problem.Problem.MOProblem` class.

Provide objectives, variables and constraints in lists.

[8]:
```
from desdeo_problem import MOProblem

prob = MOProblem(objectives=[f1_2, f3], variables=variables, constraints=[cons1])
```

The problem class provides abstractions such as the `evaluate` method. The method evaluates all the objective and constraint values for a given set of decision variables (in a numpy array), using the evaluators.

The abstraction also provides methods such as `train` and `surrogate_evaluate` for data driven problem. These will be tackled in the next notebook.

The output is a NamedTuple object. It contains the following elements:

1. `objectives`: Contains the objective values
2. `fitness`: Contains the fitness values. Fitness is either equal to the objective value, or equal to (-1 * objective value), depending upon whether the objective is to be minimized or maximized respectively. The optimization methods in the DESDEO framework internally use this value, rather than the values contained in output.objectives
3. `constraints`: Contains constraint violation values.
4. `uncertainity`: Contains the quantification of "uncertainity" of the evaluation

All of these values can be accessed in different ways, as shown below.

Note: Input as list of lists is not supported

[9]:
```
data = np.asarray([[1, -1, 0], [5, 5, 2]])
res= prob.evaluate(data)
```

[10]:
```
print(res)
# Note the sign reversal in the third objective and third fitness values because of␣
↪maximization.
```

```
Evaluation Results Object
Objective values are:
[[ 0. 12. -1.]
 [ 0. 50. 27.]]
Constraint violation values are:
[[10.]
 [-2.]]
Fitness values are:
[[  0.  12.   1.]
 [  0.  50. -27.]]
Uncertainity values are:
```

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```
[[nan nan nan]
 [nan nan nan]]
```

[11]:
```
print("The objective values for the given set of decision variables are: \n", res.
↪objectives)
print("The constraint violation for the given set of decision variables are:\n", res.
↪constraints)
```

```
The objective values for the given set of decision variables are:
 [[ 0. 12. -1.]
 [ 0. 50. 27.]]
The constraint violation for the given set of decision variables are:
 [[10.]
 [-2.]]
```

[12]:
```
res
```

[12]:
```
EvaluationResults(objectives=array([[ 0., 12., -1.],
       [ 0., 50., 27.]]), fitness=array([[  0.,  12.,   1.],
       [  0.,  50., -27.]]), constraints=array([[10.],
       [-2.]]), uncertainity=array([[nan, nan, nan],
       [nan, nan, nan]]))
```

[ ]:
```

```

How to make and use the test problems

Currently supported: * ZDT Problems- ZDT1-4, ZDT6 * DTLZ Problems- DTLZ1-7

Import the test problem builder

[1]:
```
from desdeo_problem.testproblems.TestProblems import test_problem_builder
```

Use `test_problem_builder` to build the necessary `MOProblem` instance, which can be used by methods in desdeo-emo and desdeo-mcdm to solve multiobjective optimization problems

[2]:
```
help(test_problem_builder)
```

```
Help on function test_problem_builder in module desdeo_problem.testproblems.
↪TestProblems:

test_problem_builder(name: str, n_of_variables: int = None, n_of_objectives: int =␣
↪None) -> desdeo_problem.problem.Problem.MOProblem
    Build test problems. Currently supported: ZDT1-4, ZDT6, and DTLZ1-7.

    Args:
        name (str): Name of the problem in all caps. For example: "ZDT1", "DTLZ4",␣
↪etc.
        n_of_variables (int, optional): Number of variables. Required for DTLZ␣
↪problems,
            but can be skipped for ZDT problems as they only support one variable␣
↪value.
        n_of_objectives (int, optional): Required for DTLZ problems,
            but can be skipped for ZDT problems as they only support one variable␣
↪value.
```

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```
    Raises:
        ProblemError: When one of many issues occur while building the MOProblem
            instance.

    Returns:
        MOProblem: The test problem object
```

[3]:
```
zdt1 = test_problem_builder("ZDT1")
zdt1
```

[3]:
```
<desdeo_problem.problem.Problem.MOProblem at 0x1f33b279ac8>
```

[4]:
```
dtlz3 = test_problem_builder("DTLZ3", n_of_objectives= 3, n_of_variables=20)
dtlz3
```

[4]:
```
<desdeo_problem.problem.Problem.MOProblem at 0x1f33b279208>
```

How to use these instances for other purposes, such as generating data:

[5]:
```
import numpy as np
```

Generate input data as desired:

[6]:
```
number_of_samples = 3
zdt_data = np.random.random((number_of_samples, 30))  # 30 is the number of variables␣
↪in the ZDT1 problem
print(zdt_data)
```

```
[[0.9566665  0.12642707 0.75401858 0.03765694 0.01986561 0.48660617
  0.49280935 0.85344899 0.27133411 0.93323257 0.84133493 0.20475801
  0.92905088 0.06490354 0.8570188  0.83492128 0.62833644 0.99593786
  0.81635487 0.82580931 0.56251793 0.97574662 0.47558831 0.3939823
  0.27397178 0.7496003  0.04909389 0.08239682 0.34656906 0.49915204]
 [0.74919761 0.28625722 0.67908382 0.6106337  0.6950148  0.25785019
  0.61746779 0.76319615 0.89890242 0.75963628 0.98161652 0.67291301
  0.79612155 0.52273917 0.20450823 0.7952598  0.60585745 0.4121897
  0.05809478 0.34800526 0.58840432 0.18724738 0.68237086 0.61657321
  0.3096879  0.32458604 0.16036243 0.82480997 0.17956196 0.01421743]
 [0.9957692  0.19364135 0.11009589 0.63606894 0.92162454 0.95342228
  0.88665615 0.74501953 0.09816078 0.48951933 0.76896919 0.64603171
  0.90088292 0.26154581 0.91006787 0.89883207 0.45426937 0.47012129
  0.01451065 0.40256939 0.2019439  0.45817166 0.56534801 0.18641038
  0.91780371 0.19666782 0.83473067 0.15496044 0.01478023 0.85545543]]
```

[7]:
```
dtlz_data = np.random.random((number_of_samples, 20)) # We put the number of␣
↪variables earlier as 20
```

`<MOProblem object>.evaluate(data)` returns a tuple containing the objective values and constraint violations

[8]:
```
zdt_obj_val = zdt1.evaluate(zdt_data)
zdt_obj_val
```

[8]:
```
EvaluationResults(objectives=array([[0.9566665 , 3.42361516],
       [0.74919761, 3.55955498],
```

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```
       [0.9957692 , 3.31853043]]), fitness=array([[0.9566665 , 3.42361516],
       [0.74919761, 3.55955498],
       [0.9957692 , 3.31853043]]), constraints=None, uncertainity=array([[nan, nan],
       [nan, nan],
       [nan, nan]]))
```

There are no constraints in the zdt or dtlz problems, hence cons_val is None

[9]:
```
dtlz_obj_val = dtlz3.evaluate(dtlz_data)
dtlz_obj_val
```

[9]:
```
EvaluationResults(objectives=array([[1307.49928399, 1214.1266996 ,  555.10066581],
       [ 248.94975775,  162.82774202, 2199.31133262],
       [1052.58290325, 1701.71639663,  600.67385014]]), fitness=array([[1307.49928399,
↪ 1214.1266996 ,  555.10066581],
       [ 248.94975775,  162.82774202, 2199.31133262],
       [1052.58290325, 1701.71639663,  600.67385014]]), constraints=None,␣
↪uncertainity=array([[nan, nan, nan],
       [nan, nan, nan],
       [nan, nan, nan]]))
```

[ ]:
```

```

Data based problem

If the problem to be optimized has already been solved for a representation of its' Pareto efficient front, it can be defined as a ScalarDataProblem.

Suppose we have a problem with 2 decision variables and 4 objectives. In this case, it is the river pollution problem as defined in https://ieeexplore.ieee.org/document/35354

The computed Pareto efficient solutions and the corresponding objective vector values have been computed in the file 'riverpollution.dat'. There is a total of 500 entries. Begin by importing relevant classes and laoding the data.

[2]:
```
# NOTE: This will soon be depreciated.
from desdeo_problem import ScalarDataProblem

import numpy as np

data = np.loadtxt("./data/riverpollution.dat")
```

The first 2 entries of each row are the decision variables, and the last 4 the objective function values.

[3]:
```
xs, fs = data[:, 0:2], data[:, 2:]
```

The problem can now be defined:

[4]:
```
problem = ScalarDataProblem(xs, fs)
```

That's it. Now the problem is defined and can be further utilized. Notice that there are no constraints. It is assumed that all the entries in the data file are feasible. The warning has to do with the fact, that the data is discrete, therefore the evaluations for specific decision variable values have to be approximated somehow. At the moment, the closest pair of decision variables is searched for in the data. Later on, a surrogate model for the data might be build to have a better approximation.

[5]:
```
print("N of objectives:", problem.n_of_objectives)
print("N of variables:", problem.n_of_variables)

print("Single decision vector evaluaion:", problem.evaluate([0.4, 0.5]))
```

```
N of objectives: 4
N of variables: 2
Single decision vector evaluaion: (array([-5.6304735 , -2.87892556, -7.06008234,  0.
↪05013393]),)
```

[ ]:
```
```

Data Based Problems

The DESDEO framework provides handling of data-driven optimization problems. Some methods, such as E-NAUTILUS in `desdeo-mcdm`, find the most preffered solution from a provided dataset. Other methods, such as most of the EA's from `desdeo-emo`, require a surrogate model to be trained for each of the objectives. The `desdeo_problem` provides support for both of these cases.

For data based problems, use the data specific objective/problem classes

[1]:
```
import pandas as pd
import numpy as np
```

VectorDataObjective is an objective class that can handle data, as well as multi-objective evaluators.

The GaussianProcessRegressor here is same as the one in scikit-learn with one small difference. The predict method has been replaced to return uncertainity values (in the form of standard deviation of the prediction) by default. It supports hyperparameters in the same format as the sklearn method.

[2]:
```
from desdeo_problem import VectorDataObjective as VDO
from desdeo_problem.surrogatemodels.SurrogateModels import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import Matern
```

Creating some random data

'a' and 'b' are randomly generated between 0 and 1.

f1 = a + b
f2 = a * b

For data-driven problems, make sure that the input dataset is in the pandas DataFrame format, with the column names being the same as the variable/objective names.

[3]:
```
data = np.random.rand(100,2)

f1 = (data[:,0]+data[:,1]).reshape(-1,1)
f2 = (data[:,0]*data[:,1]).reshape(-1,1)

data = np.hstack((data, f1, f2))
```

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```
X = ['a','b']
y = ['f1','f2']
datapd = pd.DataFrame(data, columns=X+y)
datapd.head()
```

[3]:

```
          a         b        f1        f2
0  0.730445  0.051709  0.782154  0.037771
1  0.039999  0.693915  0.733915  0.027756
2  0.024957  0.584356  0.609313  0.014584
3  0.774647  0.427847  1.202494  0.331430
4  0.500549  0.012714  0.513263  0.006364
```

Using VectorDataObjective class

The `VectorDataObjective` class takes as its input the data in a dataframe format and the objective names in a list.

[4]:

```
obj = VDO(data=datapd, name=y)
```

Training surrogate models

Pass the surrogate modelling technique and the model parameters to the train method of the objective instance.

If only one modelling technique is passed, the `model_parameters` should be a dict (or None) and this will be used for all the objectives.

If multiple modelling techniques are passed, `models` should be the list of modelling techniques, and `model_parameters` should be a list of dicts. The length of these lists should be the same as the number of objectives and each list element will be used to train one objective in order.

[5]:

```
obj.train(models=GaussianProcessRegressor, model_parameters={'kernel': Matern(nu=1.5)}
↪)
```

Using surrogate models to evaluate objective values

Use the obj.evaluate method to get predictions. Note that `use_surrogates` should be true.

[6]:

```
print(obj.evaluate(np.asarray([[0.5,0.3]]), use_surrogate=True))
```

```
Objective Evaluation Results Object
Objective values are:
         f1        f2
0  0.800011  0.150043
Uncertainity values are:
         f1        f2
0  0.000615  0.001536
```

[7]:

```
obj._model_trained
```

[7]:

```
{'f1': True, 'f2': True}
```

Creating data problem class

Creating the objective class should be bypassed for now, use `DataProblem` class directly with the data in a dataframe.

The `DataProblem` provides a `train` method which trains all the objectives sequentially. The input arguments for this train method is the same as that of the `VectorDataObjective` class.

To make sure that the `evaluate` method uses the surrogate models for evaluations, pass the `use_surrogate=True` argument.

[8]:
```
from desdeo_problem import DataProblem
```

[9]:
```
maximize = pd.DataFrame([[True, False]], columns=['f1','f2'])
prob = DataProblem(data=datapd, objective_names=y, variable_names=X,␣
↪maximize=maximize)
```

[10]:
```
prob.train(GaussianProcessRegressor)
```

[11]:
```
print(prob.evaluate(np.asarray([[0.1,0.8], [0.5,0.3]]), use_surrogate=True))
```

```
Evaluation Results Object
Objective values are:
[[0.89999924 0.08000021]
 [0.8        0.14999895]]
Constraint violation values are:
None
Fitness values are:
[[-0.89999924  0.08000021]
 [-0.8         0.14999895]]
Uncertainity values are:
[[0.00346248 0.00346248]
 [0.00374312 0.00374312]]
```

Lipschitian models

[12]:
```
from desdeo_problem.surrogatemodels.lipschitzian import LipschitzianRegressor
```

[13]:
```
prob = DataProblem(data=datapd, objective_names=y, variable_names=X)
```

[14]:
```
prob.train(LipschitzianRegressor)
```

[15]:
```
print(prob.evaluate(np.asarray([[0.1,0.8], [0.5,0.3]]), use_surrogate=True))
```

```
Evaluation Results Object
Objective values are:
[[0.9        0.08734629]
 [0.8        0.16056562]]
Constraint violation values are:
None
Fitness values are:
[[0.9        0.08734629]
 [0.8        0.16056562]]
```

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```
Uncertainity values are:
[[3.33066907e-16 1.74576926e-02]
 [6.10622664e-16 7.72293212e-02]]
```

[ ]:

How to use Lipschitzian modelling

[1]:
```
import numpy as np
import pandas as pd
from desdeo_problem.surrogatemodels.lipschitzian import LipschitzianRegressor
import matplotlib.pyplot as plt
```

[2]:
```
def y_func(x):
    return(np.sin(x) + np.sin(2*x))
```

[3]:
```
num_points = 20
x = np.linspace(0, 2 * np.pi, num_points).reshape(-1,1)
y = y_func(x)
data = pd.DataFrame(np.hstack((x,y)), columns = ['x','y'])
```

[4]:
```
model = LipschitzianRegressor()
```

[5]:
```
model.fit(X=data['x'], y = data['y'])
```

[6]:
```
model.L
```

[6]:
```
2.8392177826759726
```

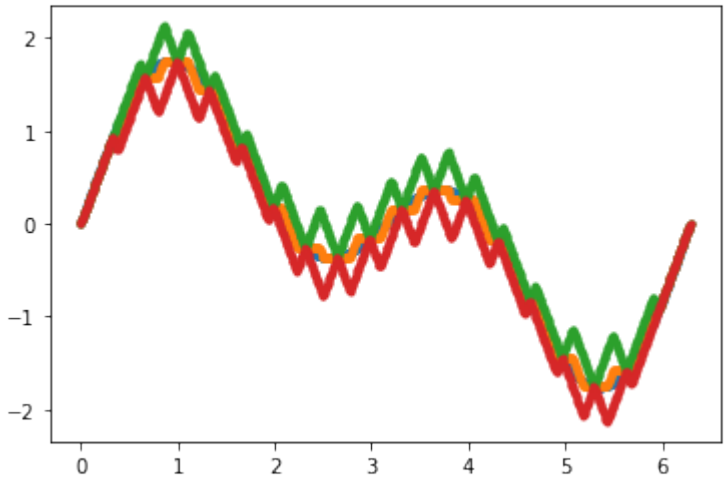
[7]:
```
model.y
```

[7]:
```
array([[ 0.00000000e+00],
       [ 9.38912182e-01],
       [ 1.58361298e+00],
       [ 1.75293980e+00],
       [ 1.44534766e+00],
       [ 8.31989903e-01],
       [ 1.80049416e-01],
       [-2.60860582e-01],
       [-3.61219085e-01],
       [-1.60104879e-01],
       [ 1.60104879e-01],
       [ 3.61219085e-01],
       [ 2.60860582e-01],
       [-1.80049416e-01],
       [-8.31989903e-01],
       [-1.44534766e+00],
       [-1.75293980e+00],
       [-1.58361298e+00],
       [-9.38912182e-01],
       [-7.34788079e-16]])
```

[8]:
```
x_new = np.linspace(0, 2*np.pi, 1000).reshape(-1,1)
y_new_true = y_func(x_new)
y_mean, y_delta = model.predict(x_new)
```

[9]:
```
plt.scatter(x_new, y_new_true, marker='.')
plt.scatter(x_new, y_mean, marker='.')
plt.scatter(x_new, y_mean + y_delta, marker='.')
plt.scatter(x_new, y_mean - y_delta, marker='.')
```

[9]:
```
<matplotlib.collections.PathCollection at 0x2c4d3b5d9c8>
```



[10]:
```
def y_func2d(x):
    return(np.sin(x[:,0]) + np.sin(2*x[:,1]))
```

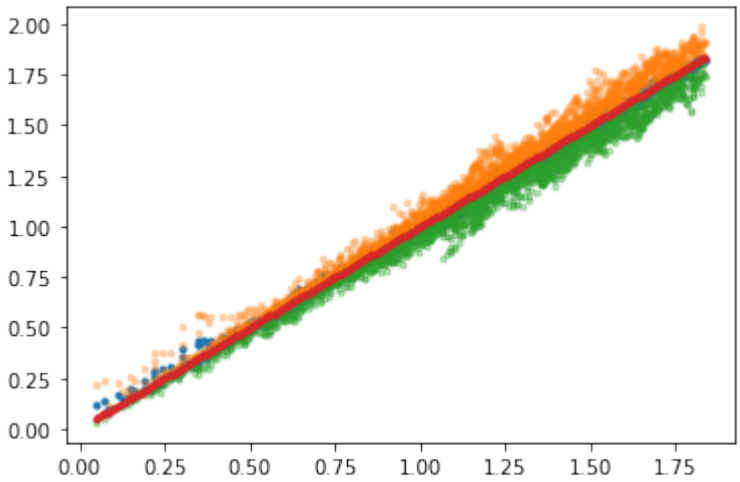
[11]:
```
x = np.random.rand(200,2)
y = y_func2d(x).reshape(-1,1)
data = pd.DataFrame(np.hstack((x,y)), columns = ['x1', 'x2','y'])
```

[12]:
```
model = LipschitzianRegressor()
model.fit(X=data[['x1', 'x2']], y = data['y'])
```

[13]:
```
x_new = np.random.rand(2000,2)
y_new_true = y_func2d(x_new).reshape(-1,1)
y_predict, y_delta = model.predict(x_new)
```

[14]:
```
line = np.linspace(y_new_true.min(),y_new_true.max(),200)
plt.scatter(y_new_true, y_predict.reshape(-1,1), marker=".")
plt.scatter(y_new_true, (y_predict+y_delta).reshape(-1,1), marker=".", alpha=0.3)
plt.scatter(y_new_true, (y_predict-y_delta).reshape(-1,1), marker=".", alpha=0.3)
plt.scatter(line,line, marker='.')
```

[14]:
```
<matplotlib.collections.PathCollection at 0x2c4d4c56c08>
```


2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75

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PYTHON MODULE INDEX

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