PyKrige Documentation

Release 1.6.1

PyKrige developers

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CONTENTS

CHAPTER

ONE

PYKRIGE

Kriging Toolkit for Python.

1.1 Purpose

The code supports 2D and 3D ordinary and universal kriging. Standard variogram models (linear, power, spherical, gaussian, exponential) are built in, but custom variogram models can also be used. The 2D universal kriging code currently supports regional-linear, point-logarithmic, and external drift terms, while the 3D universal kriging code supports a regional-linear drift term in all three spatial dimensions. Both universal kriging classes also support generic 'specified' and 'functional' drift capabilities. With the 'specified' drift capability, the user may manually specify the values of the drift(s) at each data point and all grid points. With the 'functional' drift capability, the user may provide callable function(s) of the spatial coordinates that define the drift(s). The package includes a module that contains functions that should be useful in working with ASCII grid files (`\*.asc`).

See the documentation at http://pykrige.readthedocs.io/ for more details and examples.

1.2 Installation

PyKrige requires Python 3.5+ as well as numpy, scipy. It can be installed from PyPi with,

```
pip install pykrige
```

scikit-learn is an optional dependency needed for parameter tuning and regression kriging. matplotlib is an optional dependency needed for plotting.

If you use conda, PyKrige can be installed from the channel with,

```
conda install -c conda-forge pykrige
```

1.3 Features

1.3.1 Kriging algorithms

- `OrdinaryKriging`: 2D ordinary kriging with estimated mean
- `UniversalKriging`: 2D universal kriging providing drift terms
- `OrdinaryKriging3D`: 3D ordinary kriging
- `UniversalKriging3D`: 3D universal kriging
- `RegressionKriging`: An implementation of Regression-Kriging
- `ClassificationKriging`: An implementation of Simplicial Indicator Kriging

1.3.2 Wrappers

- `rk.Krige`: A scikit-learn wrapper class for Ordinary and Universal Kriging

1.3.3 Tools

- `kriging_tools.write_asc_grid`: Writes gridded data to ASCII grid file (`\*.asc`)
- `kriging_tools.read_asc_grid`: Reads ASCII grid file (`\*.asc`)
- `kriging_tools.write_zmap_grid`: Writes gridded data to zmap file (`\*.zmap`)
- `kriging_tools.read_zmap_grid`: Reads zmap file (`\*.zmap`)

1.3.4 Kriging Parameters Tuning

A scikit-learn compatible API for parameter tuning by cross-validation is exposed in sklearn.model_selection.GridSearchCV. See the Krige CV example for a more practical illustration.

1.3.5 Regression Kriging

Regression kriging can be performed with pykrige.rk.RegressionKriging. This class takes as parameters a scikit-learn regression model, and details of either the `OrdinaryKriging` or the `UniversalKriging` class, and performs a correction step on the ML regression prediction.

A demonstration of the regression kriging is provided in the corresponding example.

1.3.6 Classification Kriging

Simplifical Indicator kriging can be performed with pykrige.ck.ClassificationKriging. This class takes as parameters a scikit-learn classification model, and details of either the `OrdinaryKriging` or the `UniversalKriging` class, and performs a correction step on the ML classification prediction.

A demonstration of the classification kriging is provided in the corresponding example.

1.4 License

PyKrige uses the BSD 3-Clause License.

CHAPTER

TWO

VARIOGRAM MODELS

PyKrige internally supports the six variogram models listed below. Additionally, the code supports user-defined variogram models via the 'custom' variogram model keyword argument.

- Gaussian Model

$$p \cdot (1 - e^{-\frac{d^2}{(\frac{4}{7}r)^2}}) + n$$

- Exponential Model

$$p \cdot (1 - e^{-\frac{d}{r/3}}) + n$$

- Spherical Model

$$\begin{cases} p \cdot (\frac{3d}{2r} - \frac{d^3}{2r^3}) + n & d \leq r \\ p + n & d > r \end{cases}$$

- Linear Model

$$s \cdot d + n$$

Where *s* is the slope and *n* is the nugget.

- Power Model

$$s \cdot d^e + n$$

Where *s* is the scaling factor, *e* is the exponent (between 0 and 2), and *n* is the nugget term.

- Hole-Effect Model

$$p \cdot (1 - (1 - \frac{d}{r/3}) * e^{-\frac{d}{r/3}}) + n$$

Variables are defined as:

d = distance values at which to calculate the variogram

p = partial sill (psill = sill - nugget)

r = range

n = nugget

s = scaling factor or slope

e = exponent for power model

For stationary variogram models (gaussian, exponential, spherical, and hole-effect models), the partial sill is defined as the difference between the full sill and the nugget term. The sill represents the asymptotic maximum spatial variance at longest lags (distances). The range represents the distance at which the spatial variance has reached ~95% of the sill variance. The nugget effectively takes up 'noise' in measurements. It represents the random deviations from an overall

smooth spatial data trend. (The name *nugget* is an allusion to kriging's mathematical origin in gold exploration; the nugget effect is intended to take into account the possibility that when sampling you randomly hit a pocket gold that is anomalously richer than the surrounding area.)

For nonstationary models (linear and power models, with unbounded spatial variances), the nugget has the same meaning. The exponent for the power-law model should be between 0 and 2[1].

A few important notes:

The PyKrige user interface by default takes the full sill. This default behavior can be changed with a keyword flag, so that the user can supply the partial sill instead. The code internally uses the partial sill (psill = sill - nugget) rather than the full sill, as it's safer to perform automatic variogram estimation using the partial sill.

The exact definitions of the variogram models here may differ from those used elsewhere. Keep that in mind when switching from another kriging code over to PyKrige.

According to[1], the hole-effect variogram model is only correct for the 1D case. It's implemented here for completeness and should be used cautiously.

2.1 References

[1] P.K. Kitanidis, Introduction to Geostatistics: Applications in Hydrogeology, (Cambridge University Press, 1997) 272 p.

CHAPTER

THREE

API REFERENCE

3.1 Krigging algorithms

pykrige.ok.OrdinaryKriging(x, y, z[, ...])	Convenience class for easy access to 2D Ordinary Kriging.
pykrige.uk.UniversalKriging(x, y, z[, ...])	Provides greater control over 2D kriging by utilizing drift terms.
pykrige.ok3d.OrdinaryKriging3D(x, y, z, val)	Three-dimensional ordinary kriging.
pykrige.uk3d.UniversalKriging3D(x, y, z, val)	Three-dimensional universal kriging.
pykrige.rk.RegressionKriging([...])	An implementation of Regression-Kriging.

3.1.1 pykrige.ok.OrdinaryKriging

class pykrige.ok.**OrdinaryKriging**(*x*, *y*, *z*, *variogram_model='linear'*, *variogram_parameters=None*, *variogram_function=None*, *nlags=6*, *weight=False*, *anisotropy_scaling=1.0*, *anisotropy_angle=0.0*, *verbose=False*, *enable_plotting=False*, *enable_statistics=False*, *coordinates_type='euclidean'*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*)

Convenience class for easy access to 2D Ordinary Kriging.

Parameters

- **x** (*array_like*) – X-coordinates of data points.
- **y** (*array_like*) – Y-coordinates of data points.
- **z** (*array-like*) – Values at data points.
- **variogram_model** (*str or GSTools CovModel, optional*) – Specifies which variogram model to use; may be one of the following: linear, power, gaussian, spherical, exponential, hole-effect. Default is linear variogram model. To utilize a custom variogram model, specify 'custom'; you must also provide variogram_parameters and variogram_function. Note that the hole-effect model is only technically correct for one-dimensional problems. You can also use a GSTools CovModel.
- **variogram_parameters** (*list or dict, optional*) – Parameters that define the specified variogram model. If not provided, parameters will be automatically calculated

using a "soft" L1 norm minimization scheme. For variogram model parameters provided in a dict, the required dict keys vary according to the specified variogram model:

```
# linear
    {'slope': slope, 'nugget': nugget}
# power
    {'scale': scale, 'exponent': exponent, 'nugget': nugget}
# gaussian, spherical, exponential and hole-effect:
    {'sill': s, 'range': r, 'nugget': n}
    # OR
    {'psill': p, 'range': r, 'nugget': n}
```

Note that either the full sill or the partial sill (psill = sill - nugget) can be specified in the dict. For variogram model parameters provided in a list, the entries must be as follows:

```
# linear
    [slope, nugget]
# power
    [scale, exponent, nugget]
# gaussian, spherical, exponential and hole-effect:
    [sill, range, nugget]
```

Note that the full sill (NOT the partial sill) must be specified in the list format. For a custom variogram model, the parameters are required, as custom variogram models will not automatically be fit to the data. Furthermore, the parameters must be specified in list format, in the order in which they are used in the callable function (see variogram_function for more information). The code does not check that the provided list contains the appropriate number of parameters for the custom variogram model, so an incorrect parameter list in such a case will probably trigger an esoteric exception someplace deep in the code. NOTE that, while the list format expects the full sill, the code itself works internally with the partial sill.

- **variogram_function** (*callable, optional*) – A callable function that must be provided if variogram_model is specified as 'custom'. The function must take only two arguments: first, a list of parameters for the variogram model; second, the distances at which to calculate the variogram model. The list provided in variogram_parameters will be passed to the function as the first argument.
- **nlags** (*int, optional*) – Number of averaging bins for the semivariogram. Default is 6.
- **weight** (*bool, optional*) – Flag that specifies if semivariance at smaller lags should be weighted more heavily when automatically calculating variogram model. The routine is currently hard-coded such that the weights are calculated from a logistic function, so weights at small lags are ~1 and weights at the longest lags are ~0; the center of the logistic weighting is hard-coded to be at 70% of the distance from the shortest lag to the largest lag. Setting this parameter to True indicates that weights will be applied. Default is False. (Kitanidis suggests that the values at smaller lags are more important in fitting a variogram model, so the option is provided to enable such weighting.)
- **anisotropy_scaling** (*float, optional*) – Scalar stretching value to take into account anisotropy. Default is 1 (effectively no stretching). Scaling is applied in the y-direction in the rotated data frame (i.e., after adjusting for the anisotropy_angle, if anisotropy_angle is not 0). This parameter has no effect if coordinate_types is set to 'geographic'.
- **anisotropy_angle** (*float, optional*) – CCW angle (in degrees) by which to rotate coordinate system in order to take into account anisotropy. Default is 0 (no rotation).

Note that the coordinate system is rotated. This parameter has no effect if coordinate_types is set to 'geographic'.

- **verbose** (*bool, optional*) – Enables program text output to monitor kriging process. Default is False (off).
- **enable_plotting** (*bool, optional*) – Enables plotting to display variogram. Default is False (off).
- **enable_statistics** (*bool, optional*) – Default is False
- **coordinates_type** (*str, optional*) – One of 'euclidean' or 'geographic'. Determines if the x and y coordinates are interpreted as on a plane ('euclidean') or as coordinates on a sphere ('geographic'). In case of geographic coordinates, x is interpreted as longitude and y as latitude coordinates, both given in degree. Longitudes are expected in [0, 360] and latitudes in [-90, 90]. Default is 'euclidean'.
- **exact_values** (*bool, optional*) – If True, interpolation provides input values at input locations. If False, interpolation accounts for variance/nugget within input values at input locations and does not behave as an exact-interpolator [2]. Note that this only has an effect if there is variance/nugget present within the input data since it is interpreted as measurement error. If the nugget is zero, the kriged field will behave as an exact interpolator.
- **pseudo_inv** (`bool`, optional) – Whether the kriging system is solved with the pseudo inverted kriging matrix. If *True*, this leads to more numerical stability and redundant points are averaged. But it can take more time. Default: False
- **pseudo_inv_type** (`str`, optional) – Here you can select the algorithm to compute the pseudo-inverse matrix:
  - *"pinv"*: use *pinv* from *scipy* which uses *lstsq*
  - *"pinv2"*: use *pinv2* from *scipy* which uses *SVD*
  - *"pinvh"*: use *pinvh* from *scipy* which uses eigen-values

  Default: *"pinv"*

References

__init__(*x*, *y*, *z*, *variogram_model='linear'*, *variogram_parameters=None*, *variogram_function=None*, *nlags=6*, *weight=False*, *anisotropy_scaling=1.0*, *anisotropy_angle=0.0*, *verbose=False*, *enable_plotting=False*, *enable_statistics=False*, *coordinates_type='euclidean'*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*)

Initialize self. See help(type(self)) for accurate signature.

Methods

`__init__`(x, y, z[, variogram_model, ...])	Initialize self.
`display_variogram_model`()	Displays variogram model with the actual binned data.
`execute`(style, xpoints, ypoints[, mask, ...])	Calculates a kriged grid and the associated variance.
`get_epsilon_residuals`()	Returns the epsilon residuals for the variogram fit.
`get_statistics`()	Returns the Q1, Q2, and cR statistics for the variogram fit (in that order).

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Table 2 – continued from previous page

get_variogram_points()	Returns both the lags and the variogram function evaluated at each of them.
plot_epsilon_residuals()	Plots the epsilon residuals for the variogram fit.
print_statistics()	Prints out the Q1, Q2, and cR statistics for the variogram fit.
switch_plotting()	Allows user to switch plot display on/off.
switch_verbose()	Allows user to switch code talk-back on/off.
update_variogram_model(variogram_model[, ...])	Allows user to update variogram type and/or variogram model parameters.

Attributes

eps
variogram_dict

3.1.2 pykrige.uk.UniversalKriging

class pykrige.uk.**UniversalKriging**(*x*, *y*, *z*, *variogram_model='linear'*, *variogram_parameters=None*, *variogram_function=None*, *nlags=6*, *weight=False*, *anisotropy_scaling=1.0*, *anisotropy_angle=0.0*, *drift_terms=None*, *point_drift=None*, *external_drift=None*, *external_drift_x=None*, *external_drift_y=None*, *specified_drift=None*, *functional_drift=None*, *verbose=False*, *enable_plotting=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*)

Provides greater control over 2D kriging by utilizing drift terms.

Parameters

- **x** (*array_like*) – X-coordinates of data points.
- **y** (*array_like*) – Y-coordinates of data points.
- **z** (*array_like*) – Values at data points.
- **variogram_model** (*str or GSTools CovModel, optional*) – Specified which variogram model to use; may be one of the following: linear, power, gaussian, spherical, exponential, hole-effect. Default is linear variogram model. To utilize a custom variogram model, specify 'custom'; you must also provide variogram_parameters and variogram_function. Note that the hole-effect model is only technically correct for one-dimensional problems. You can also use a GSTools CovModel.
- **variogram_parameters** (*list or dict, optional*) – Parameters that define the specified variogram model. If not provided, parameters will be automatically calculated using a "soft" L1 norm minimization scheme. For variogram model parameters provided in a dict, the required dict keys vary according to the specified variogram model:

```
# linear
    {'slope': slope, 'nugget': nugget}
# power
```

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```
    {'scale': scale, 'exponent': exponent, 'nugget': nugget}
# gaussian, spherical, exponential and hole-effect:
    {'sill': s, 'range': r, 'nugget': n}
    # OR
    {'psill': p, 'range': r, 'nugget': n}
```

Note that either the full sill or the partial sill (psill = sill - nugget) can be specified in the dict. For variogram model parameters provided in a list, the entries must be as follows:

```
# linear
    [slope, nugget]
# power
    [scale, exponent, nugget]
# gaussian, spherical, exponential and hole-effect:
    [sill, range, nugget]
```

Note that the full sill (NOT the partial sill) must be specified in the list format. For a custom variogram model, the parameters are required, as custom variogram models will not automatically be fit to the data. Furthermore, the parameters must be specified in list format, in the order in which they are used in the callable function (see variogram_function for more information). The code does not check that the provided list contains the appropriate number of parameters for the custom variogram model, so an incorrect parameter list in such a case will probably trigger an esoteric exception someplace deep in the code. NOTE that, while the list format expects the full sill, the code itself works internally with the partial sill.

- **variogram_function** (*callable, optional*) – A callable function that must be provided if variogram_model is specified as 'custom'. The function must take only two arguments: first, a list of parameters for the variogram model; second, the distances at which to calculate the variogram model. The list provided in variogram_parameters will be passed to the function as the first argument.
- **nlags** (*int, optional*) – Number of averaging bins for the semivariogram. Default is 6.
- **weight** (*bool, optional*) – Flag that specifies if semivariance at smaller lags should be weighted more heavily when automatically calculating variogram model. The routine is currently hard-coded such that the weights are calculated from a logistic function, so weights at small lags are ~1 and weights at the longest lags are ~0; the center of the logistic weighting is hard-coded to be at 70% of the distance from the shortest lag to the largest lag. Setting this parameter to True indicates that weights will be applied. Default is False. (Kitanidis suggests that the values at smaller lags are more important in fitting a variogram model, so the option is provided to enable such weighting.)
- **anisotropy_scaling** (*float, optional*) – Scalar stretching value to take into account anisotropy. Default is 1 (effectively no stretching). Scaling is applied in the y-direction in the rotated data frame (i.e., after adjusting for the anisotropy_angle, if anisotropy_angle is not 0).
- **anisotropy_angle** (*float, optional*) – CCW angle (in degrees) by which to rotate coordinate system in order to take into account anisotropy. Default is 0 (no rotation). Note that the coordinate system is rotated.
- **drift_terms** (*list of strings, optional*) – List of drift terms to include in universal kriging. Supported drift terms are currently 'regional_linear', 'point_log', 'external_Z', 'specified', and 'functional'.
- **point_drift** (*array_like, optional*) – Array-like object that contains the coor-

dinates and strengths of the point-logarithmic drift terms. Array shape must be (N, 3), where N is the number of point drift terms. First column (index 0) must contain x-coordinates, second column (index 1) must contain y-coordinates, and third column (index 2) must contain the strengths of each point term. Strengths are relative, so only the relation of the values to each other matters. Note that the code will appropriately deal with point-logarithmic terms that are at the same coordinates as an evaluation point or data point, but Python will still kick out a warning message that an ln(0) has been encountered. If the problem involves anisotropy, the well coordinates will be adjusted and the drift values will be calculated in the adjusted data frame.

- **external_drift** (*array_like, optional*) – Gridded data used for the external Z scalar drift term. Must be shape (M, N), where M is in the y-direction and N is in the x-direction. Grid spacing does not need to be constant. If grid spacing is not constant, must specify the grid cell sizes. If the problem involves anisotropy, the external drift values are extracted based on the pre-adjusted coordinates (i.e., the original coordinate system).
- **external_drift_x** (*array_like, optional*) – X-coordinates for gridded external Z-scalar data. Must be shape (M,) or (M, 1), where M is the number of grid cells in the x-direction. The coordinate is treated as the center of the cell.
- **external_drift_y** (*array_like, optional*) – Y-coordinates for gridded external Z-scalar data. Must be shape (N,) or (N, 1), where N is the number of grid cells in the y-direction. The coordinate is treated as the center of the cell.
- **specified_drift** (*list of array-like objects, optional*) – List of arrays that contain the drift values at data points. The arrays must be shape (N,) or (N, 1), where N is the number of data points. Any number of specified-drift terms may be used.
- **functional_drift** (*list of callable objects, optional*) – List of callable functions that will be used to evaluate drift terms. The function must be a function of only the two spatial coordinates and must return a single value for each coordinate pair. It must be set up to be called with only two arguments, first an array of x values and second an array of y values. If the problem involves anisotropy, the drift values are calculated in the adjusted data frame.
- **verbose** (*bool, optional*) – Enables program text output to monitor kriging process. Default is False (off).
- **enable_plotting** (*boolean, optional*) – Enables plotting to display variogram. Default is False (off).
- **exact_values** (*bool, optional*) – If True, interpolation provides input values at input locations. If False, interpolation accounts for variance/nugget within input values at input locations and does not behave as an exact-interpolator [2]. Note that this only has an effect if there is variance/nugget present within the input data since it is interpreted as measurement error. If the nugget is zero, the kriged field will behave as an exact interpolator.
- **pseudo_inv** (`bool`, optional) – Whether the kriging system is solved with the pseudo inverted kriging matrix. If *True*, this leads to more numerical stability and redundant points are averaged. But it can take more time. Default: False
- **pseudo_inv_type** (`str`, optional) – Here you can select the algorithm to compute the pseudo-inverse matrix:
  - *"pinv"*: use *pinv* from *scipy* which uses *lstsq*
  - *"pinv2"*: use *pinv2* from *scipy* which uses *SVD*
  - *"pinvh"*: use *pinvh* from *scipy* which uses eigen-values

  Default: *"pinv"*

References

__init__(*x*, *y*, *z*, *variogram_model='linear'*, *variogram_parameters=None*, *variogram_function=None*, *nlags=6*, *weight=False*, *anisotropy_scaling=1.0*, *anisotropy_angle=0.0*, *drift_terms=None*, *point_drift=None*, *external_drift=None*, *external_drift_x=None*, *external_drift_y=None*, *specified_drift=None*, *functional_drift=None*, *verbose=False*, *enable_plotting=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*)

Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(x, y, z[, variogram_model, ...])	Initialize self.
display_variogram_model()	Displays variogram model with the actual binned data.
execute(style, xpoints, ypoints[, mask, ...])	Calculates a kriged grid and the associated variance.
get_epsilon_residuals()	Returns the epsilon residuals for the variogram fit.
get_statistics()	Returns the Q1, Q2, and cR statistics for the variogram fit (in that order).
get_variogram_points()	Returns both the lags and the variogram function evaluated at each of them.
plot_epsilon_residuals()	Plots the epsilon residuals for the variogram fit.
print_statistics()	Prints out the Q1, Q2, and cR statistics for the variogram fit.
switch_plotting()	Allows user to switch plot display on/off.
switch_verbose()	Allows user to switch code talk-back on/off.
update_variogram_model(variogram_model[, ...])	Allows user to update variogram type and/or variogram model parameters.

Attributes

UNBIAS
eps
variogram_dict

3.1.3 pykrige.ok3d.OrdinaryKriging3D

class pykrige.ok3d.**OrdinaryKriging3D**(*x*, *y*, *z*, *val*, *variogram_model='linear'*, *variogram_parameters=None*, *variogram_function=None*, *nlags=6*, *weight=False*, *anisotropy_scaling_y=1.0*, *anisotropy_scaling_z=1.0*, *anisotropy_angle_x=0.0*, *anisotropy_angle_y=0.0*, *anisotropy_angle_z=0.0*, *verbose=False*, *enable_plotting=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*)

Three-dimensional ordinary kriging.

Parameters

- **x** (*array_like*) – X-coordinates of data points.
- **y** (*array_like*) – Y-coordinates of data points.
- **z** (*array_like*) – Z-coordinates of data points.
- **val** (*array_like*) – Values at data points.
- **variogram_model** (*str or GSTools CovModel, optional*) – Specified which variogram model to use; may be one of the following: linear, power, gaussian, spherical, exponential, hole-effect. Default is linear variogram model. To utilize a custom variogram model, specify 'custom'; you must also provide variogram_parameters and variogram_function. Note that the hole-effect model is only technically correct for one-dimensional problems. You can also use a GSTools CovModel.
- **variogram_parameters** (*list or dict, optional*) – Parameters that define the specified variogram model. If not provided, parameters will be automatically calculated using a "soft" L1 norm minimization scheme. For variogram model parameters provided in a dict, the required dict keys vary according to the specified variogram model:

```
# linear
    {'slope': slope, 'nugget': nugget}
# power
    {'scale': scale, 'exponent': exponent, 'nugget': nugget}
# gaussian, spherical, exponential and hole-effect:
    {'sill': s, 'range': r, 'nugget': n}
    # OR
    {'psill': p, 'range': r, 'nugget': n}
```

Note that either the full sill or the partial sill (psill = sill - nugget) can be specified in the dict. For variogram model parameters provided in a list, the entries must be as follows:

```
# linear
    [slope, nugget]
# power
    [scale, exponent, nugget]
# gaussian, spherical, exponential and hole-effect:
    [sill, range, nugget]
```

Note that the full sill (NOT the partial sill) must be specified in the list format. For a custom variogram model, the parameters are required, as custom variogram models will not automatically be fit to the data. Furthermore, the parameters must be specified in list format, in the order in which they are used in the callable function (see variogram_function for more information). The code does not check that the provided list contains the appropriate number of parameters for the custom variogram model, so an incorrect parameter list in such a case will probably trigger an esoteric exception someplace deep in the code. NOTE that, while the list format expects the full sill, the code itself works internally with the partial sill.

- **variogram_function** (*callable, optional*) – A callable function that must be provided if variogram_model is specified as 'custom'. The function must take only two arguments: first, a list of parameters for the variogram model; second, the distances at which to calculate the variogram model. The list provided in variogram_parameters will be passed to the function as the first argument.
- **nlags** (*int, optional*) – Number of averaging bins for the semivariogram. Default is 6.

- **weight** (*boolean, optional*) – Flag that specifies if semivariance at smaller lags should be weighted more heavily when automatically calculating variogram model. The routine is currently hard-coded such that the weights are calculated from a logistic function, so weights at small lags are ~1 and weights at the longest lags are ~0; the center of the logistic weighting is hard-coded to be at 70% of the distance from the shortest lag to the largest lag. Setting this parameter to True indicates that weights will be applied. Default is False. (Kitanidis suggests that the values at smaller lags are more important in fitting a variogram model, so the option is provided to enable such weighting.)
- **anisotropy_scaling_y** (*float, optional*) – Scalar stretching value to take into account anisotropy in the y direction. Default is 1 (effectively no stretching). Scaling is applied in the y direction in the rotated data frame (i.e., after adjusting for the anisotropy_angle_x/y/z, if anisotropy_angle_x/y/z is/are not 0).
- **anisotropy_scaling_z** (*float, optional*) – Scalar stretching value to take into account anisotropy in the z direction. Default is 1 (effectively no stretching). Scaling is applied in the z direction in the rotated data frame (i.e., after adjusting for the anisotropy_angle_x/y/z, if anisotropy_angle_x/y/z is/are not 0).
- **anisotropy_angle_x** (*float, optional*) – CCW angle (in degrees) by which to rotate coordinate system about the x axis in order to take into account anisotropy. Default is 0 (no rotation). Note that the coordinate system is rotated. X rotation is applied first, then y rotation, then z rotation. Scaling is applied after rotation.
- **anisotropy_angle_y** (*float, optional*) – CCW angle (in degrees) by which to rotate coordinate system about the y axis in order to take into account anisotropy. Default is 0 (no rotation). Note that the coordinate system is rotated. X rotation is applied first, then y rotation, then z rotation. Scaling is applied after rotation.
- **anisotropy_angle_z** (*float, optional*) – CCW angle (in degrees) by which to rotate coordinate system about the z axis in order to take into account anisotropy. Default is 0 (no rotation). Note that the coordinate system is rotated. X rotation is applied first, then y rotation, then z rotation. Scaling is applied after rotation.
- **verbose** (*bool, optional*) – Enables program text output to monitor kriging process. Default is False (off).
- **enable_plotting** (*bool, optional*) – Enables plotting to display variogram. Default is False (off).
- **exact_values** (*bool, optional*) – If True, interpolation provides input values at input locations. If False, interpolation accounts for variance/nugget within input values at input locations and does not behave as an exact-interpolator [2]. Note that this only has an effect if there is variance/nugget present within the input data since it is interpreted as measurement error. If the nugget is zero, the kriged field will behave as an exact interpolator.
- **pseudo_inv** (`bool`, optional) – Whether the kriging system is solved with the pseudo inverted kriging matrix. If *True*, this leads to more numerical stability and redundant points are averaged. But it can take more time. Default: False
- **pseudo_inv_type** (`str`, optional) – Here you can select the algorithm to compute the pseudo-inverse matrix:
  - *"pinv"*: use *pinv* from *scipy* which uses *lstsq*
  - *"pinv2"*: use *pinv2* from *scipy* which uses *SVD*
  - *"pinvh"*: use *pinvh* from *scipy* which uses eigen-values

  Default: *"pinv"*

References

__init__(*x*, *y*, *z*, *val*, *variogram_model='linear'*, *variogram_parameters=None*, *variogram_function=None*, *nlags=6*, *weight=False*, *anisotropy_scaling_y=1.0*, *anisotropy_scaling_z=1.0*, *anisotropy_angle_x=0.0*, *anisotropy_angle_y=0.0*, *anisotropy_angle_z=0.0*, *verbose=False*, *enable_plotting=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(x, y, z, val[, variogram_model, ...])	Initialize self.
display_variogram_model()	Displays variogram model with the actual binned data.
execute(style, xpoints, ypoints, zpoints[, ...])	Calculates a kriged grid and the associated variance.
get_epsilon_residuals()	Returns the epsilon residuals for the variogram fit.
get_statistics()	Returns the Q1, Q2, and cR statistics for the variogram fit (in that order).
plot_epsilon_residuals()	Plots the epsilon residuals for the variogram fit.
print_statistics()	Prints out the Q1, Q2, and cR statistics for the variogram fit.
switch_plotting()	Allows user to switch plot display on/off.
switch_verbose()	Allows user to switch code talk-back on/off.
update_variogram_model(variogram_model[, ...])	Changes the variogram model and variogram parameters for the kriging system.

Attributes

eps
variogram_dict

3.1.4 pykrige.uk3d.UniversalKriging3D

class pykrige.uk3d.**UniversalKriging3D**(*x*, *y*, *z*, *val*, *variogram_model='linear'*, *variogram_parameters=None*, *variogram_function=None*, *nlags=6*, *weight=False*, *anisotropy_scaling_y=1.0*, *anisotropy_scaling_z=1.0*, *anisotropy_angle_x=0.0*, *anisotropy_angle_y=0.0*, *anisotropy_angle_z=0.0*, *drift_terms=None*, *specified_drift=None*, *functional_drift=None*, *verbose=False*, *enable_plotting=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*)
Three-dimensional universal kriging.

Parameters

- **x** (*array_like*) – X-coordinates of data points.

- **y** (*array_like*) – Y-coordinates of data points.
- **z** (*array_like*) – Z-coordinates of data points.
- **val** (*array_like*) – Values at data points.
- **variogram_model** (*str or GSTools CovModel, optional*) – Specified which variogram model to use; may be one of the following: linear, power, gaussian, spherical, exponential, hole-effect. Default is linear variogram model. To utilize a custom variogram model, specify 'custom'; you must also provide variogram_parameters and variogram_function. Note that the hole-effect model is only technically correct for one-dimensional problems. You can also use a GSTools CovModel.
- **variogram_parameters** (*list or dict, optional*) – Parameters that define the specified variogram model. If not provided, parameters will be automatically calculated using a "soft" L1 norm minimization scheme. For variogram model parameters provided in a dict, the required dict keys vary according to the specified variogram model:

```
# linear
    {'slope': slope, 'nugget': nugget}
# power
    {'scale': scale, 'exponent': exponent, 'nugget': nugget}
# gaussian, spherical, exponential and hole-effect:
    {'sill': s, 'range': r, 'nugget': n}
    # OR
    {'psill': p, 'range': r, 'nugget': n}
```

Note that either the full sill or the partial sill (psill = sill - nugget) can be specified in the dict. For variogram model parameters provided in a list, the entries must be as follows:

```
# linear
    [slope, nugget]
# power
    [scale, exponent, nugget]
# gaussian, spherical, exponential and hole-effect:
    [sill, range, nugget]
```

Note that the full sill (NOT the partial sill) must be specified in the list format. For a custom variogram model, the parameters are required, as custom variogram models will not automatically be fit to the data. Furthermore, the parameters must be specified in list format, in the order in which they are used in the callable function (see variogram_function for more information). The code does not check that the provided list contains the appropriate number of parameters for the custom variogram model, so an incorrect parameter list in such a case will probably trigger an esoteric exception someplace deep in the code. NOTE that, while the list format expects the full sill, the code itself works internally with the partial sill.

- **variogram_function** (*callable, optional*) – A callable function that must be provided if variogram_model is specified as 'custom'. The function must take only two arguments: first, a list of parameters for the variogram model; second, the distances at which to calculate the variogram model. The list provided in variogram_parameters will be passed to the function as the first argument.
- **nlags** (*int, optional*) – Number of averaging bins for the semivariogram. Default is 6.
- **weight** (*bool, optional*) – Flag that specifies if semivariance at smaller lags should be weighted more heavily when automatically calculating variogram model. The routine is currently hard-coded such that the weights are calculated from a logistic function, so weights at small lags are ~1 and weights at the longest lags are ~0; the center of the logistic

weighting is hard-coded to be at 70% of the distance from the shortest lag to the largest lag. Setting this parameter to True indicates that weights will be applied. Default is False. (Kitanidis suggests that the values at smaller lags are more important in fitting a variogram model, so the option is provided to enable such weighting.)

- **anisotropy_scaling_y** (*float, optional*) – Scalar stretching value to take into account anisotropy in the y direction. Default is 1 (effectively no stretching). Scaling is applied in the y direction in the rotated data frame (i.e., after adjusting for the anisotropy_angle_x/y/z, if anisotropy_angle_x/y/z is/are not 0).
- **anisotropy_scaling_z** (*float, optional*) – Scalar stretching value to take into account anisotropy in the z direction. Default is 1 (effectively no stretching). Scaling is applied in the z direction in the rotated data frame (i.e., after adjusting for the anisotropy_angle_x/y/z, if anisotropy_angle_x/y/z is/are not 0).
- **anisotropy_angle_x** (*float, optional*) – CCW angle (in degrees) by which to rotate coordinate system about the x axis in order to take into account anisotropy. Default is 0 (no rotation). Note that the coordinate system is rotated. X rotation is applied first, then y rotation, then z rotation. Scaling is applied after rotation.
- **anisotropy_angle_y** (*float, optional*) – CCW angle (in degrees) by which to rotate coordinate system about the y axis in order to take into account anisotropy. Default is 0 (no rotation). Note that the coordinate system is rotated. X rotation is applied first, then y rotation, then z rotation. Scaling is applied after rotation.
- **anisotropy_angle_z** (*float, optional*) – CCW angle (in degrees) by which to rotate coordinate system about the z axis in order to take into account anisotropy. Default is 0 (no rotation). Note that the coordinate system is rotated. X rotation is applied first, then y rotation, then z rotation. Scaling is applied after rotation.
- **drift_terms** (*list of strings, optional*) – List of drift terms to include in three-dimensional universal kriging. Supported drift terms are currently 'regional_linear', 'specified', and 'functional'.
- **specified_drift** (*list of array-like objects, optional*) – List of arrays that contain the drift values at data points. The arrays must be shape (N,) or (N, 1), where N is the number of data points. Any number of specified-drift terms may be used.
- **functional_drift** (*list of callable objects, optional*) – List of callable functions that will be used to evaluate drift terms. The function must be a function of only the three spatial coordinates and must return a single value for each coordinate triplet. It must be set up to be called with only three arguments, first an array of x values, the second an array of y values, and the third an array of z values. If the problem involves anisotropy, the drift values are calculated in the adjusted data frame.
- **verbose** (*boolean, optional*) – Enables program text output to monitor kriging process. Default is False (off).
- **enable_plotting** (*boolean, optional*) – Enables plotting to display variogram. Default is False (off).
- **exact_values** (*bool, optional*) – If True, interpolation provides input values at input locations. If False, interpolation accounts for variance/nugget within input values at input locations and does not behave as an exact-interpolator [2]. Note that this only has an effect if there is variance/nugget present within the input data since it is interpreted as measurement error. If the nugget is zero, the kriged field will behave as an exact interpolator.
- **pseudo_inv** (bool, optional) – Whether the kriging system is solved with the pseudo inverted kriging matrix. If *True*, this leads to more numerical stability and redundant points are averaged. But it can take more time. Default: False

- **pseudo_inv_type** (str, optional) – Here you can select the algorithm to compute the pseudo-inverse matrix:
  - *"pinv"*: use *pinv* from *scipy* which uses *lstsq*
  - *"pinv2"*: use *pinv2* from *scipy* which uses *SVD*
  - *"pinvh"*: use *pinvh* from *scipy* which uses eigen-values

  Default: *"pinv"*

References

__init__(*x*, *y*, *z*, *val*, *variogram_model='linear'*, *variogram_parameters=None*, *variogram_function=None*, *nlags=6*, *weight=False*, *anisotropy_scaling_y=1.0*, *anisotropy_scaling_z=1.0*, *anisotropy_angle_x=0.0*, *anisotropy_angle_y=0.0*, *anisotropy_angle_z=0.0*, *drift_terms=None*, *specified_drift=None*, *functional_drift=None*, *verbose=False*, *enable_plotting=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*)

Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(x, y, z, val[, variogram_model, ...])	Initialize self.
display_variogram_model()	Displays semivariogram and variogram model.
execute(style, xpoints, ypoints, zpoints[, ...])	Calculates a kriged grid and the associated variance.
get_epsilon_residuals()	Returns the epsilon residuals for the variogram fit.
get_statistics()	Returns the Q1, Q2, and cR statistics for the variogram fit (in that order).
plot_epsilon_residuals()	Plots the epsilon residuals for the variogram fit.
print_statistics()	Prints out the Q1, Q2, and cR statistics for the variogram fit.
switch_plotting()	Enables/disable variogram plot display.
switch_verbose()	Enables/disables program text output.
update_variogram_model(variogram_model[, ...])	Changes the variogram model and variogram parameters for the kriging system.

Attributes

UNBIAS
eps
variogram_dict

3.1.5 pykrige.rk.RegressionKriging

class pykrige.rk.**RegressionKriging**(*regression_model=SVR()*, *method='ordinary'*, *variogram_model='linear'*, *n_closest_points=10*, *nlags=6*, *weight=False*, *verbose=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*, *variogram_parameters=None*, *variogram_function=None*, *anisotropy_scaling=(1.0, 1.0)*, *anisotropy_angle=(0.0, 0.0, 0.0)*, *enable_statistics=False*, *coordinates_type='euclidean'*, *drift_terms=None*, *point_drift=None*, *ext_drift_grid=(None, None, None)*, *functional_drift=None*)

An implementation of Regression-Kriging.

As described here: https://en.wikipedia.org/wiki/Regression-Kriging

Parameters

- **regression_model** (*machine learning model instance from sklearn*) –
- **method** (*str, optional*) – type of kriging to be performed
- **variogram_model** (*str, optional*) – variogram model to be used during Kriging
- **n_closest_points** (*int*) – number of closest points to be used during Ordinary Kriging
- **nlags** (*int*) – see OK/UK class description
- **weight** (*bool*) – see OK/UK class description
- **verbose** (*bool*) – see OK/UK class description
- **exact_values** (*bool*) – see OK/UK class description
- **variogram_parameters** (*list or dict*) – see OK/UK class description
- **variogram_function** (*callable*) – see OK/UK class description
- **anisotropy_scaling** (*tuple*) – single value for 2D (UK/OK) and two values in 3D (UK3D/OK3D)
- **anisotropy_angle** (*tuple*) – single value for 2D (UK/OK) and three values in 3D (UK3D/OK3D)
- **enable_statistics** (*bool*) – see OK class description
- **coordinates_type** (*str*) – see OK/UK class description
- **drift_terms** (*list of strings*) – see UK/UK3D class description
- **point_drift** (*array_like*) – see UK class description
- **ext_drift_grid** (*tuple*) – Holding the three values external_drift, external_drift_x and external_drift_z for the UK class
- **functional_drift** (*list of callable*) – see UK/UK3D class description

__init__(*regression_model=SVR()*, *method='ordinary'*, *variogram_model='linear'*, *n_closest_points=10*, *nlags=6*, *weight=False*, *verbose=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*, *variogram_parameters=None*, *variogram_function=None*, *anisotropy_scaling=(1.0, 1.0)*, *anisotropy_angle=(0.0, 0.0, 0.0)*, *enable_statistics=False*, *coordinates_type='euclidean'*, *drift_terms=None*, *point_drift=None*, *ext_drift_grid=(None, None, None)*, *functional_drift=None*)

Initialize self. See help(type(self)) for accurate signature.

Methods

`__init__`([regression_model, method, ...])	Initialize self.
`fit`(p, x, y)	Fit the regression method and also Krige the residual.
`krige_residual`(x, **kwargs)	Calculate the residuals.
`predict`(p, x, **kwargs)	Predict.
`score`(p, x, y[, sample_weight])	Overloading default regression score method.

3.2 Wrappers

`pykrige.rk.Krige`([method, variogram_model, ...])	A scikit-learn wrapper class for Ordinary and Universal Kriging.

3.2.1 pykrige.rk.Krige

class pykrige.rk.**Krige**(*method='ordinary'*, *variogram_model='linear'*, *nlags=6*, *weight=False*, *n_closest_points=10*, *verbose=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*, *variogram_parameters=None*, *variogram_function=None*, *anisotropy_scaling=(1.0, 1.0)*, *anisotropy_angle=(0.0, 0.0, 0.0)*, *enable_statistics=False*, *coordinates_type='euclidean'*, *drift_terms=None*, *point_drift=None*, *ext_drift_grid=(None, None, None)*, *functional_drift=None*)

A scikit-learn wrapper class for Ordinary and Universal Kriging.

This works with both Grid/RandomSearchCv for finding the best Krige parameters combination for a problem.

Parameters

- **method** (*str, optional*) – type of kriging to be performed
- **variogram_model** (*str, optional*) – variogram model to be used during Kriging
- **nlags** (*int*) – see OK/UK class description
- **weight** (*bool*) – see OK/UK class description
- **n_closest_points** (*int*) – number of closest points to be used during Ordinary Kriging
- **verbose** (*bool*) – see OK/UK class description
- **exact_values** (*bool*) – see OK/UK class description
- **variogram_parameters** (*list or dict*) – see OK/UK class description
- **variogram_function** (*callable*) – see OK/UK class description
- **anisotropy_scaling** (*tuple*) – single value for 2D (UK/OK) and two values in 3D (UK3D/OK3D)
- **anisotropy_angle** (*tuple*) – single value for 2D (UK/OK) and three values in 3D (UK3D/OK3D)

- **enable_statistics** (*bool*) – see OK class description
- **coordinates_type** (*str*) – see OK/UK class description
- **drift_terms** (*list of strings*) – see UK/UK3D class description
- **point_drift** (*array_like*) – see UK class description
- **ext_drift_grid** (*tuple*) – Holding the three values external_drift, external_drift_x and external_drift_z for the UK class
- **functional_drift** (*list of callable*) – see UK/UK3D class description

__init__(*method='ordinary'*, *variogram_model='linear'*, *nlags=6*, *weight=False*, *n_closest_points=10*, *verbose=False*, *exact_values=True*, *pseudo_inv=False*, *pseudo_inv_type='pinv'*, *variogram_parameters=None*, *variogram_function=None*, *anisotropy_scaling=(1.0, 1.0)*, *anisotropy_angle=(0.0, 0.0, 0.0)*, *enable_statistics=False*, *coordinates_type='euclidean'*, *drift_terms=None*, *point_drift=None*, *ext_drift_grid=(None, None, None)*, *functional_drift=None*)

Initialize self. See help(type(self)) for accurate signature.

Methods

__init__([method, variogram_model, nlags, ...])	Initialize self.
execute(points, *args, **kwargs)	Execute.
fit(x, y, *args, **kwargs)	Fit the current model.
get_params([deep])	Get parameters for this estimator.
predict(x, *args, **kwargs)	Predict.
score(X, y[, sample_weight])	Return the coefficient of determination R^2 of the prediction.
set_params(**params)	Set the parameters of this estimator.

3.3 Tools

pykrige.kriging_tools.write_asc_grid(x, y, z)	Writes gridded data to ASCII grid file (*.asc).
pykrige.kriging_tools.read_asc_grid(filename)	Reads ASCII grid file (*.asc).

3.3.1 pykrige.kriging_tools.write_asc_grid

pykrige.kriging_tools.**write_asc_grid**(*x*, *y*, *z*, *filename='output.asc'*, *no_data=-999.0*, *style=1*)

Writes gridded data to ASCII grid file (*.asc).

This is useful for exporting data to a GIS program.

Parameters

- **x** (*array_like, shape (N,) or (N, 1)*) – X-coordinates of grid points at center of cells.
- **y** (*array_like, shape (M,) or (M, 1)*) – Y-coordinates of grid points at center of cells.

- **z** (*array_like, shape (M, N)*) – Gridded data values. May be a masked array.
- **filename** (*string, optional*) – Name of output *.asc file. Default name is 'output.asc'.
- **no_data** (*float, optional*) – no data value to be used
- **style** (*int, optional*) – Determines how to write the *.asc file header. Specifying 1 writes out DX, DY, XLLCENTER, YLLCENTER. Specifying 2 writes out CELLSIZE (note DX must be the same as DY), XLLCORNER, YLLCORNER. Default is 1.

3.3.2 pykrige.kriging_tools.read_asc_grid

pykrige.kriging_tools.**read_asc_grid**(*filename*, *footer=0*)

Reads ASCII grid file (*.asc).

Parameters

- **filename** (*str*) – Name of *.asc file.
- **footer** (*int, optional*) – Number of lines at bottom of *.asc file to skip.

Returns

- **grid_array** (*numpy array, shape (M, N)*) – (M, N) array of grid values, where M is number of Y-coordinates and N is number of X-coordinates. The array entry corresponding to the lower-left coordinates is at index [M, 0], so that the array is oriented as it would be in X-Y space.
- **x** (*numpy array, shape (N,)*) – 1D array of N X-coordinates.
- **y** (*numpy array, shape (M,)*) – 1D array of M Y-coordinates.
- **CELLSIZE** (*tuple or float*) – Either a two-tuple of (x-cell size, y-cell size), or a float that specifies the uniform cell size.
- **NODATA** (*float*) – Value that specifies which entries are not actual data.

CHAPTER

FOUR

EXAMPLES

4.1 Universal Kriging Example

In this example we apply a regional linear trend to the kriging system.

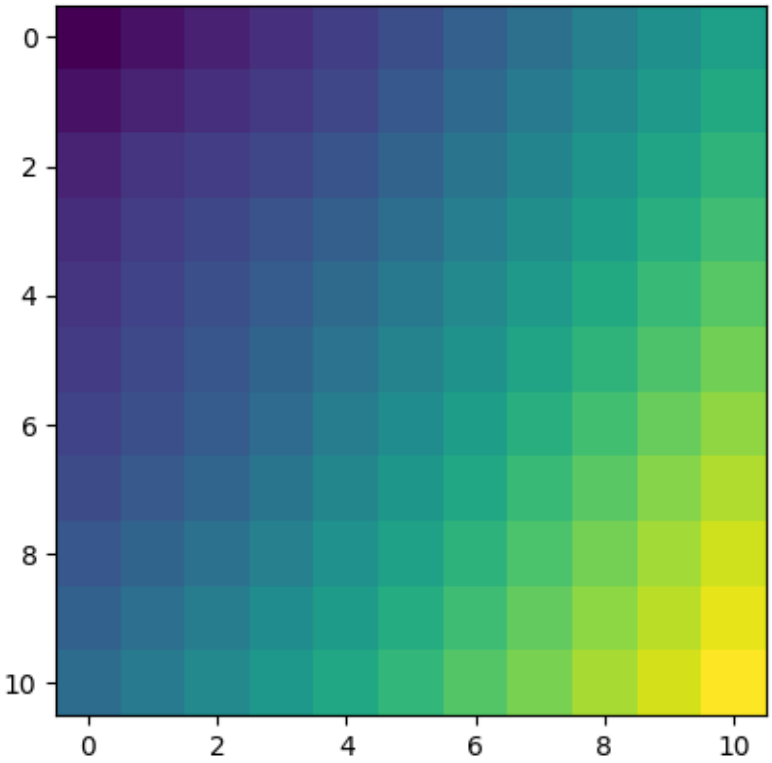
```
from pykrige.uk import UniversalKriging
import numpy as np
import matplotlib.pyplot as plt


data = np.array(
    [
        [0.3, 1.2, 0.47],
        [1.9, 0.6, 0.56],
        [1.1, 3.2, 0.74],
        [3.3, 4.4, 1.47],
        [4.7, 3.8, 1.74],
    ]
)

gridx = np.arange(0.0, 5.5, 0.5)
gridy = np.arange(0.0, 5.5, 0.5)
```

Create the universal kriging object. Required inputs are the X-coordinates of the data points, the Y-coordinates of the data points, and the Z-values of the data points. Variogram is handled as in the ordinary kriging case. drift_terms is a list of the drift terms to include; currently supported terms are 'regional_linear', 'point_log', and 'external_Z'. Refer to UniversalKriging.__doc__ for more information.

```
UK = UniversalKriging(
    data[:, 0],
    data[:, 1],
    data[:, 2],
    variogram_model="linear",
    drift_terms=["regional_linear"],
)
```

Creates the kriged grid and the variance grid. Allows for kriging on a rectangular grid of points, on a masked rectangular grid of points, or with arbitrary points. (See UniversalKriging.__doc__ for more information.)

```
z, ss = UK.execute("grid", gridx, gridy)
plt.imshow(z)
plt.show()
```



Total running time of the script: (0 minutes 0.165 seconds)

4.2 Ordinary Kriging Example

First we will create a 2D dataset together with the associated x, y grids.

```
import numpy as np
import pykrige.kriging_tools as kt
from pykrige.ok import OrdinaryKriging
import matplotlib.pyplot as plt


data = np.array(
    [
        [0.3, 1.2, 0.47],
        [1.9, 0.6, 0.56],
        [1.1, 3.2, 0.74],
        [3.3, 4.4, 1.47],
        [4.7, 3.8, 1.74],
    ]
)

gridx = np.arange(0.0, 5.5, 0.5)
gridy = np.arange(0.0, 5.5, 0.5)
```

Create the ordinary kriging object. Required inputs are the X-coordinates of the data points, the Y-coordinates of the data points, and the Z-values of the data points. If no variogram model is specified, defaults to a linear variogram model. If no variogram model parameters are specified, then the code automatically calculates the parameters by fitting the variogram model to the binned experimental semivariogram. The verbose kwarg controls code talk-back, and the enable_plotting kwarg controls the display of the semivariogram.

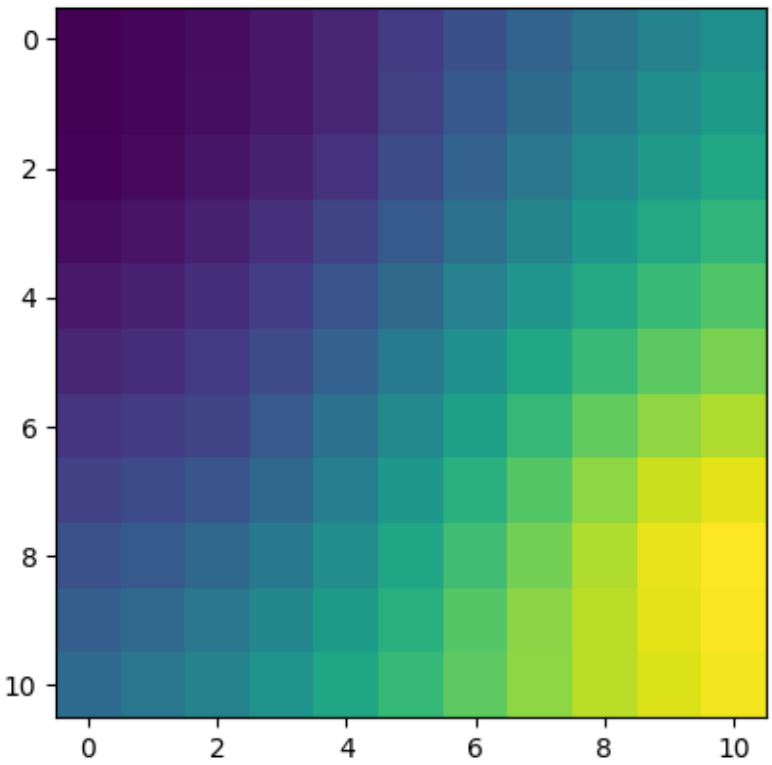
```
OK = OrdinaryKriging(
    data[:, 0],
    data[:, 1],
    data[:, 2],
    variogram_model="linear",
    verbose=False,
    enable_plotting=False,
)
```

Creates the kriged grid and the variance grid. Allows for kriging on a rectangular grid of points, on a masked rectangular grid of points, or with arbitrary points. (See OrdinaryKriging.__doc__ for more information.)

```
z, ss = OK.execute("grid", gridx, gridy)
```

Writes the kriged grid to an ASCII grid file and plot it.

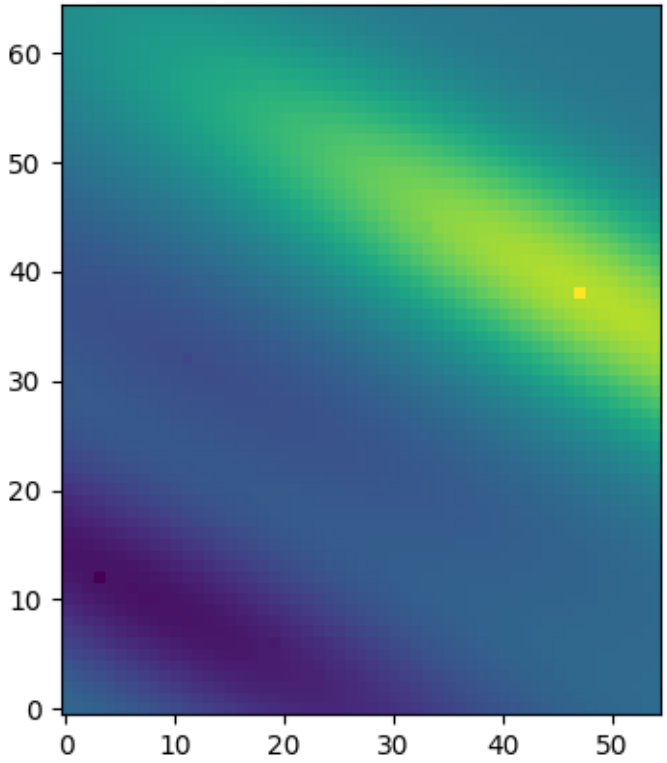
```
kt.write_asc_grid(gridx, gridy, z, filename="output.asc")
plt.imshow(z)
plt.show()
```



Total running time of the script: (0 minutes 0.144 seconds)

4.3 GSTools Interface

Example how to use the PyKrige routines with a GSTools CovModel.




```
import numpy as np
from pykrige.ok import OrdinaryKriging
from matplotlib import pyplot as plt
import gstools as gs

# conditioning data
data = np.array(
    [
        [0.3, 1.2, 0.47],
        [1.9, 0.6, 0.56],
        [1.1, 3.2, 0.74],
        [3.3, 4.4, 1.47],
        [4.7, 3.8, 1.74],
    ]
)
# grid definition for output field
gridx = np.arange(0.0, 5.5, 0.1)
```

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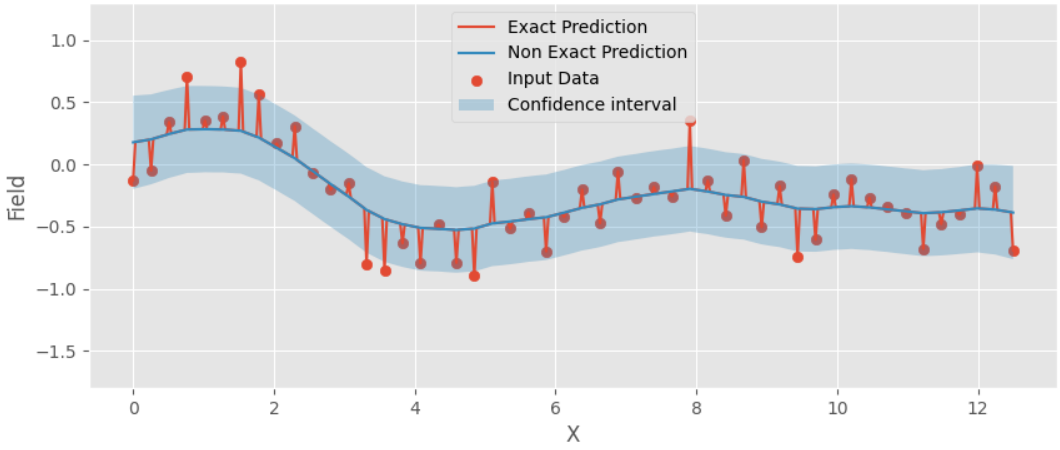
```
gridy = np.arange(0.0, 6.5, 0.1)
# a GSTools based covariance model
cov_model = gs.Gaussian(dim=2, len_scale=4, anis=0.2, angles=-0.5, var=0.5, nugget=0.
↪1)
# ordinary kriging with pykrige
OK1 = OrdinaryKriging(data[:, 0], data[:, 1], data[:, 2], cov_model)
z1, ss1 = OK1.execute("grid", gridx, gridy)
plt.imshow(z1, origin="lower")
plt.show()
```

Total running time of the script: (0 minutes 0.935 seconds)

4.4 Exact Values

PyKrige demonstration and usage as a non-exact interpolator in 1D.




```
from pykrige.ok import OrdinaryKriging
import matplotlib.pyplot as plt
import numpy as np

plt.style.use("ggplot")

np.random.seed(42)

x = np.linspace(0, 12.5, 50)
xpred = np.linspace(0, 12.5, 393)
y = np.sin(x) * np.exp(-0.25 * x) + np.random.normal(-0.25, 0.25, 50)

# compare OrdinaryKriging as an exact and non exact interpolator
uk = OrdinaryKriging(
    x, np.zeros(x.shape), y, variogram_model="linear", exact_values=False
)
uk_exact = OrdinaryKriging(x, np.zeros(x.shape), y, variogram_model="linear")

y_pred, y_std = uk.execute("grid", xpred, np.array([0.0]), backend="loop")
y_pred_exact, y_std_exact = uk_exact.execute(
```

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```
    "grid", xpred, np.array([0.0]), backend="loop"
)


y_pred = np.squeeze(y_pred)
y_std = np.squeeze(y_std)

y_pred_exact = np.squeeze(y_pred_exact)
y_std_exact = np.squeeze(y_std_exact)


fig, ax = plt.subplots(1, 1, figsize=(10, 4))

ax.scatter(x, y, label="Input Data")
ax.plot(xpred, y_pred_exact, label="Exact Prediction")
ax.plot(xpred, y_pred, label="Non Exact Prediction")

ax.fill_between(
    xpred,
    y_pred - 3 * y_std,
    y_pred + 3 * y_std,
    alpha=0.3,
    label="Confidence interval",
)
ax.legend(loc=9)
ax.set_ylim(-1.8, 1.3)
ax.legend(loc=9)
plt.xlabel("X")
plt.ylabel("Field")
plt.show()
```

Total running time of the script: (0 minutes 0.268 seconds)

4.5 Regression kriging

An example of regression kriging

Out:

```
========================================
regression model: SVR
Finished learning regression model
Finished kriging residuals
Regression Score:  -0.03405385545698292
RK score:  0.6706182225388981
========================================
regression model: RandomForestRegressor
Finished learning regression model
Finished kriging residuals
Regression Score:  0.7033047459432076
RK score:  0.7412602330513829
========================================
regression model: LinearRegression
Finished learning regression model
Finished kriging residuals
```

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```
Regression Score:  0.5277968398381674
RK score:  0.6036605153133717
```

```
import sys

from sklearn.svm import SVR
from sklearn.ensemble import RandomForestRegressor
from sklearn.linear_model import LinearRegression
from sklearn.datasets import fetch_california_housing
from sklearn.model_selection import train_test_split

from pykrige.rk import RegressionKriging

svr_model = SVR(C=0.1, gamma="auto")
rf_model = RandomForestRegressor(n_estimators=100)
lr_model = LinearRegression(normalize=True, copy_X=True, fit_intercept=False)

models = [svr_model, rf_model, lr_model]

try:
    housing = fetch_california_housing()
except PermissionError:
    # this dataset can occasionally fail to download on Windows
    sys.exit(0)

# take the first 5000 as Kriging is memory intensive
p = housing["data"][:5000, :-2]
x = housing["data"][:5000, -2:]
target = housing["target"][:5000]

p_train, p_test, x_train, x_test, target_train, target_test = train_test_split(
    p, x, target, test_size=0.3, random_state=42
)

for m in models:
    print("=" * 40)
    print("regression model:", m.__class__.__name__)
    m_rk = RegressionKriging(regression_model=m, n_closest_points=10)
    m_rk.fit(p_train, x_train, target_train)
    print("Regression Score: ", m_rk.regression_model.score(p_test, target_test))
    print("RK score: ", m_rk.score(p_test, x_test, target_test))
```

Total running time of the script: (0 minutes 7.354 seconds)

4.6 Classification kriging

An example of classification kriging

Out:

```
========================================
classification model: SVC
Finished learning classification model
Finished kriging residuals
Classification Score:  0.212
CK score:  0.6566666666666666
========================================
classification model: RandomForestClassifier
Finished learning classification model
Finished kriging residuals
Classification Score:  0.5766666666666667
CK score:  0.5946666666666667
========================================
classification model: LogisticRegression
/home/docs/checkouts/readthedocs.org/user_builds/pykrige/envs/v1.6.1/lib/python3.7/
↪site-packages/sklearn/linear_model/_logistic.py:765: ConvergenceWarning: lbfgs␣
↪failed to converge (status=1):
STOP: TOTAL NO. of ITERATIONS REACHED LIMIT.

Increase the number of iterations (max_iter) or scale the data as shown in:
    https://scikit-learn.org/stable/modules/preprocessing.html
Please also refer to the documentation for alternative solver options:
    https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression
  extra_warning_msg=_LOGISTIC_SOLVER_CONVERGENCE_MSG)
Finished learning classification model
Finished kriging residuals
Classification Score:  0.5193333333333333
CK score:  0.6553333333333333
```

```
import sys

from sklearn.svm import SVC
from sklearn.ensemble import RandomForestClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.datasets import fetch_california_housing
from sklearn.preprocessing import KBinsDiscretizer
from sklearn.model_selection import train_test_split

from pykrige.ck import ClassificationKriging

svc_model = SVC(C=0.1, gamma="auto", probability=True)
rf_model = RandomForestClassifier(n_estimators=100)
lr_model = LogisticRegression(max_iter=10000)

models = [svc_model, rf_model, lr_model]
```

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```
try:
    housing = fetch_california_housing()
except PermissionError:
    # this dataset can occasionally fail to download on Windows
    sys.exit(0)

# take the first 5000 as Kriging is memory intensive
p = housing["data"][:5000, :-2]
x = housing["data"][:5000, -2:]
target = housing["target"][:5000]
discretizer = KBinsDiscretizer(encode="ordinal")
target = discretizer.fit_transform(target.reshape(-1, 1))

p_train, p_test, x_train, x_test, target_train, target_test = train_test_split(
    p, x, target, test_size=0.3, random_state=42
)

for m in models:
    print("=" * 40)
    print("classification model:", m.__class__.__name__)
    m_ck = ClassificationKriging(classification_model=m, n_closest_points=10)
    m_ck.fit(p_train, x_train, target_train)
    print(
        "Classification Score: ", m_ck.classification_model.score(p_test, target_test)
    )
    print("CK score: ", m_ck.score(p_test, x_test, target_test))
```

Total running time of the script: (0 minutes 28.788 seconds)

4.7 Geometric example

A small example script showing the usage of the 'geographic' coordinates type for ordinary kriging on a sphere.

```
from pykrige.ok import OrdinaryKriging
import numpy as np
from matplotlib import pyplot as plt


# Make this example reproducible:
np.random.seed(89239413)

# Generate random data following a uniform spatial distribution
# of nodes and a uniform distribution of values in the interval
# [2.0, 5.5]:
N = 7
lon = 360.0 * np.random.random(N)
lat = 180.0 / np.pi * np.arcsin(2 * np.random.random(N) - 1)
z = 3.5 * np.random.rand(N) + 2.0

# Generate a regular grid with 60° longitude and 30° latitude steps:
grid_lon = np.linspace(0.0, 360.0, 7)
grid_lat = np.linspace(-90.0, 90.0, 7)

# Create ordinary kriging object:
```

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```
OK = OrdinaryKriging(
    lon,
    lat,
    z,
    variogram_model="linear",
    verbose=False,
    enable_plotting=False,
    coordinates_type="geographic",
)

# Execute on grid:
z1, ss1 = OK.execute("grid", grid_lon, grid_lat)

# Create ordinary kriging object ignoring curvature:
OK = OrdinaryKriging(
    lon, lat, z, variogram_model="linear", verbose=False, enable_plotting=False
)

# Execute on grid:
z2, ss2 = OK.execute("grid", grid_lon, grid_lat)
```

Print data at equator (last longitude index will show periodicity):

```
print("Original data:")
print("Longitude:", lon.astype(int))
print("Latitude: ", lat.astype(int))
print("z:        ", np.array_str(z, precision=2))
print("\nKrige at 60° latitude:\n======================")
print("Longitude:", grid_lon)
print("Value:    ", np.array_str(z1[5, :], precision=2))
print("Sigma²:   ", np.array_str(ss1[5, :], precision=2))
print("\nIgnoring curvature:\n====================")
print("Value:    ", np.array_str(z2[5, :], precision=2))
print("Sigma²:   ", np.array_str(ss2[5, :], precision=2))
```

Out:

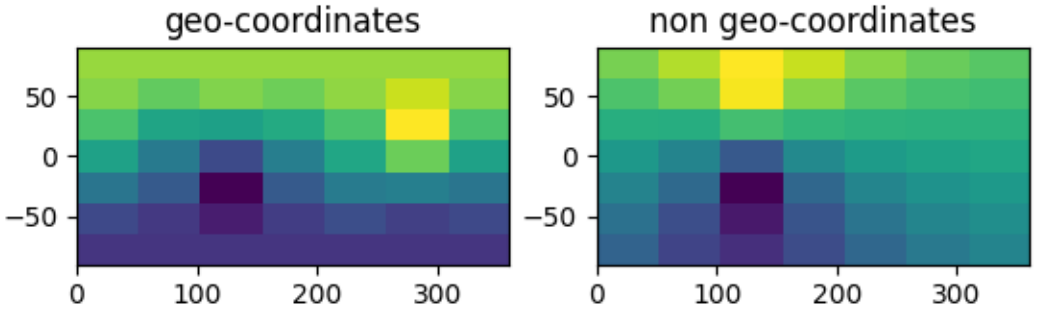
```
Original data:
Longitude: [122 166  92 138  86 122 136]
Latitude:  [-46 -36 -25 -73 -25  50 -29]
z:         [2.75 3.36 2.24 3.07 3.37 5.25 2.82]

Krige at 60° latitude:
======================
Longitude: [  0.  60. 120. 180. 240. 300. 360.]
Value:     [5.29 5.11 5.27 5.17 5.35 5.63 5.29]
Sigma²:    [2.22 1.32 0.42 1.21 2.07 2.48 2.22]

Ignoring curvature:
====================
Value:     [4.55 4.72 5.25 4.82 4.61 4.53 4.48]
Sigma²:    [3.79 2.   0.39 1.85 3.54 5.46 7.53]
```

We can see that the data point at longitude 122, latitude 50 correctly dominates the kriged results, since it is the closest node in spherical distance metric, as longitude differences scale with cos(latitude). When kriging using longitude / latitude linearly, the value for grid points with longitude values further away as longitude is now incorrectly weighted equally as latitude.

```
fig, (ax1, ax2) = plt.subplots(1, 2)
ax1.imshow(z1, extent=[0, 360, -90, 90], origin="lower")
ax1.set_title("geo-coordinates")
ax2.imshow(z2, extent=[0, 360, -90, 90], origin="lower")
ax2.set_title("non geo-coordinates")
plt.show()
```



Total running time of the script: (0 minutes 0.173 seconds)

4.8 Three-Dimensional Kriging Example

```
from pykrige.ok3d import OrdinaryKriging3D
from pykrige.uk3d import UniversalKriging3D
import numpy as np
from matplotlib import pyplot as plt


data = np.array(
    [
        [0.1, 0.1, 0.3, 0.9],
        [0.2, 0.1, 0.4, 0.8],
        [0.1, 0.3, 0.1, 0.9],
        [0.5, 0.4, 0.4, 0.5],
```

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```
        [0.3, 0.3, 0.2, 0.7],
    ]
)

gridx = np.arange(0.0, 0.6, 0.05)
gridy = np.arange(0.0, 0.6, 0.01)
gridz = np.arange(0.0, 0.6, 0.1)
```

Create the 3D ordinary kriging object and solves for the three-dimension kriged volume and variance. Refer to OrdinaryKriging3D.__doc__ for more information.

```
ok3d = OrdinaryKriging3D(
    data[:, 0], data[:, 1], data[:, 2], data[:, 3], variogram_model="linear"
)
k3d1, ss3d = ok3d.execute("grid", gridx, gridy, gridz)
```

Create the 3D universal kriging object and solves for the three-dimension kriged volume and variance. Refer to UniversalKriging3D.__doc__ for more information.

```
uk3d = UniversalKriging3D(
    data[:, 0],
    data[:, 1],
    data[:, 2],
    data[:, 3],
    variogram_model="linear",
    drift_terms=["regional_linear"],
)
k3d2, ss3d = uk3d.execute("grid", gridx, gridy, gridz)
```

To use the generic 'specified' drift term, the user must provide the drift values at each data point and at every grid point. The following example is equivalent to using a linear drift in all three spatial dimensions. Refer to UniversalKriging3D.__doc__ for more information.

```
zg, yg, xg = np.meshgrid(gridz, gridy, gridx, indexing="ij")
uk3d = UniversalKriging3D(
    data[:, 0],
    data[:, 1],
    data[:, 2],
    data[:, 3],
    variogram_model="linear",
    drift_terms=["specified"],
    specified_drift=[data[:, 0], data[:, 1], data[:, 2]],
)
k3d3, ss3d = uk3d.execute(
    "grid", gridx, gridy, gridz, specified_drift_arrays=[xg, yg, zg]
)
```

To use the generic 'functional' drift term, the user must provide a callable function that takes only the spatial dimensions as arguments. The following example is equivalent to using a linear drift only in the x-direction. Refer to UniversalKriging3D.__doc__ for more information.

```
func = lambda x, y, z: x
uk3d = UniversalKriging3D(
    data[:, 0],
    data[:, 1],
    data[:, 2],
```

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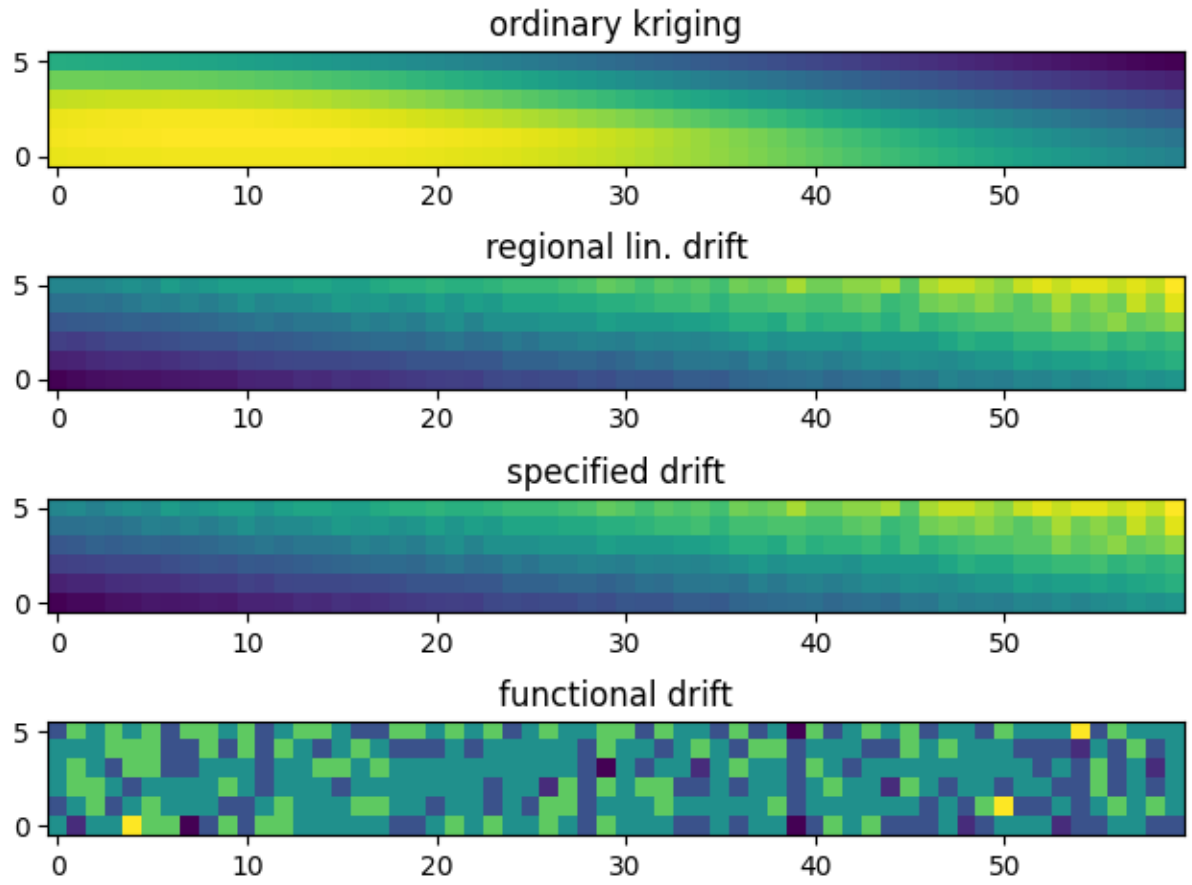
```
    data[:, 3],
    variogram_model="linear",
    drift_terms=["functional"],
    functional_drift=[func],
)
k3d4, ss3d = uk3d.execute("grid", gridx, gridy, gridz)
```

Note that the use of the 'specified' and 'functional' generic drift capabilities is essentially identical in the two-dimensional universal kriging class (except for a difference in the number of spatial coordinates for the passed drift functions). See UniversalKriging.__doc__ for more information.

```
fig, (ax1, ax2, ax3, ax4) = plt.subplots(4)
ax1.imshow(k3d1[:, :, 0], origin="lower")
ax1.set_title("ordinary kriging")
ax2.imshow(k3d2[:, :, 0], origin="lower")
ax2.set_title("regional lin. drift")
ax3.imshow(k3d3[:, :, 0], origin="lower")
ax3.set_title("specified drift")
ax4.imshow(k3d4[:, :, 0], origin="lower")
ax4.set_title("functional drift")
plt.tight_layout()
plt.show()
```



Total running time of the script: (0 minutes 0.384 seconds)

4.9 Krige CV

Searching for optimal kriging parameters with cross validation

Out:

```
Fitting 5 folds for each of 8 candidates, totalling 40 fits
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
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n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
best_score R^2 = -0.045
best_params =  {'method': 'universal', 'variogram_model': 'spherical'}

CV results::
 - mean_test_score : [-0.16726998 -0.16726998 -0.17314638 -0.15665013 -0.05679591 -0.
↪05679591
 -0.05353148 -0.04486488]
 - mean_train_score : [1. 1. 1. 1. 1. 1. 1. 1.]
 - param_method : ['ordinary' 'ordinary' 'ordinary' 'ordinary' 'universal' 'universal'
 'universal' 'universal']
```

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```
 - param_variogram_model : ['linear' 'power' 'gaussian' 'spherical' 'linear' 'power'
↪'gaussian'
 'spherical']
Fitting 5 folds for each of 8 candidates, totalling 40 fits
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
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n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
n_closest_points will be ignored for UniversalKriging
best_score R² = -0.097
best_params =  {'method': 'universal3d', 'variogram_model': 'power'}

CV results::
 - mean_test_score : [-0.25558626 -0.25299609 -0.27162923 -0.26476051 -0.11692599 -0.
↪09740764
 -0.15085041 -0.12875737]
 - mean_train_score : [1. 1. 1. 1. 1. 1. 1. 1.]
 - param_method : ['ordinary3d' 'ordinary3d' 'ordinary3d' 'ordinary3d' 'universal3d'
 'universal3d' 'universal3d' 'universal3d']
 - param_variogram_model : ['linear' 'power' 'gaussian' 'spherical' 'linear' 'power'
↪'gaussian'
 'spherical']
```

```
import numpy as np
from pykrige.rk import Krige
from sklearn.model_selection import GridSearchCV


# 2D Kring param opt

param_dict = {
    "method": ["ordinary", "universal"],
    "variogram_model": ["linear", "power", "gaussian", "spherical"],
    # "nlags": [4, 6, 8],
    # "weight": [True, False]
}

estimator = GridSearchCV(Krige(), param_dict, verbose=True, return_train_score=True)

# dummy data
X = np.random.randint(0, 400, size=(100, 2)).astype(float)
y = 5 * np.random.rand(100)

# run the gridsearch
estimator.fit(X=X, y=y)


if hasattr(estimator, "best_score_"):
    print("best_score R$^2$ = {:.3f}".format(estimator.best_score_))
    print("best_params = ", estimator.best_params_)

print("\nCV results::")
if hasattr(estimator, "cv_results_"):
    for key in [
        "mean_test_score",
        "mean_train_score",
        "param_method",
        "param_variogram_model",
    ]:
        print(" - {} : {}".format(key, estimator.cv_results_[key]))

# 3D Kring param opt

param_dict3d = {
    "method": ["ordinary3d", "universal3d"],
    "variogram_model": ["linear", "power", "gaussian", "spherical"],
    # "nlags": [4, 6, 8],
    # "weight": [True, False]
}

estimator = GridSearchCV(Krige(), param_dict3d, verbose=True, return_train_score=True)

# dummy data
X3 = np.random.randint(0, 400, size=(100, 3)).astype(float)
y = 5 * np.random.rand(100)

# run the gridsearch
```

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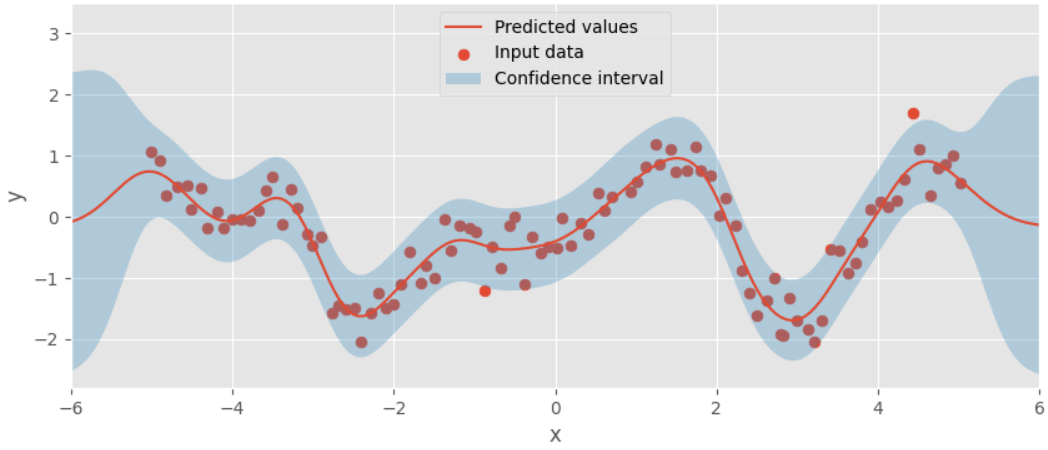
```
estimator.fit(X=X3, y=y)


if hasattr(estimator, "best_score_"):
    print("best_score R$^2$ = {:.3f}".format(estimator.best_score_))
    print("best_params = ", estimator.best_params_)

print("\nCV results::")
if hasattr(estimator, "cv_results_"):
    for key in [
        "mean_test_score",
        "mean_train_score",
        "param_method",
        "param_variogram_model",
    ]:
        print(" - {} : {}".format(key, estimator.cv_results_[key]))
```

Total running time of the script: (0 minutes 5.561 seconds)

4.10 1D Kriging

An example of 1D kriging with PyKrige




```
import numpy as np
import matplotlib.pyplot as plt
from pykrige import OrdinaryKriging

plt.style.use("ggplot")

# fmt: off
# Data taken from
# https://blog.dominodatalab.com/fitting-gaussian-process-models-python/
X, y = np.array([
     [-5.01, 1.06], [-4.90, 0.92], [-4.82, 0.35], [-4.69, 0.49], [-4.56, 0.52],
     [-4.52, 0.12], [-4.39, 0.47], [-4.32,-0.19], [-4.19, 0.08], [-4.11,-0.19],
     [-4.00,-0.03], [-3.89,-0.03], [-3.78,-0.05], [-3.67, 0.10], [-3.59, 0.44],
```

(continues on next page)

(continued from previous page)

```
    [-3.50, 0.66], [-3.39,-0.12], [-3.28, 0.45], [-3.20, 0.14], [-3.07,-0.28],
    [-3.01,-0.46], [-2.90,-0.32], [-2.77,-1.58], [-2.69,-1.44], [-2.60,-1.51],
    [-2.49,-1.50], [-2.41,-2.04], [-2.28,-1.57], [-2.19,-1.25], [-2.10,-1.50],
    [-2.00,-1.42], [-1.91,-1.10], [-1.80,-0.58], [-1.67,-1.08], [-1.61,-0.79],
    [-1.50,-1.00], [-1.37,-0.04], [-1.30,-0.54], [-1.19,-0.15], [-1.06,-0.18],
    [-0.98,-0.25], [-0.87,-1.20], [-0.78,-0.49], [-0.68,-0.83], [-0.57,-0.15],
    [-0.50, 0.00], [-0.38,-1.10], [-0.29,-0.32], [-0.18,-0.60], [-0.09,-0.49],
    [0.03 ,-0.50], [0.09 ,-0.02], [0.20 ,-0.47], [0.31 ,-0.11], [0.41 ,-0.28],
    [0.53 , 0.40], [0.61 , 0.11], [0.70 , 0.32], [0.94 , 0.42], [1.02 , 0.57],
    [1.13 , 0.82], [1.24 , 1.18], [1.30 , 0.86], [1.43 , 1.11], [1.50 , 0.74],
    [1.63 , 0.75], [1.74 , 1.15], [1.80 , 0.76], [1.93 , 0.68], [2.03 , 0.03],
    [2.12 , 0.31], [2.23 ,-0.14], [2.31 ,-0.88], [2.40 ,-1.25], [2.50 ,-1.62],
    [2.63 ,-1.37], [2.72 ,-0.99], [2.80 ,-1.92], [2.83 ,-1.94], [2.91 ,-1.32],
    [3.00 ,-1.69], [3.13 ,-1.84], [3.21 ,-2.05], [3.30 ,-1.69], [3.41 ,-0.53],
    [3.52 ,-0.55], [3.63 ,-0.92], [3.72 ,-0.76], [3.80 ,-0.41], [3.91 , 0.12],
    [4.04 , 0.25], [4.13 , 0.16], [4.24 , 0.26], [4.32 , 0.62], [4.44 , 1.69],
    [4.52 , 1.11], [4.65 , 0.36], [4.74 , 0.79], [4.84 , 0.87], [4.93 , 1.01],
    [5.02 , 0.55]
]).T
# fmt: on

X_pred = np.linspace(-6, 6, 200)

# pykrige doesn't support 1D data for now, only 2D or 3D
# adapting the 1D input to 2D
uk = OrdinaryKriging(X, np.zeros(X.shape), y, variogram_model="gaussian")

y_pred, y_std = uk.execute("grid", X_pred, np.array([0.0]))

y_pred = np.squeeze(y_pred)
y_std = np.squeeze(y_std)

fig, ax = plt.subplots(1, 1, figsize=(10, 4))
ax.scatter(X, y, s=40, label="Input data")


ax.plot(X_pred, y_pred, label="Predicted values")
ax.fill_between(
    X_pred,
    y_pred - 3 * y_std,
    y_pred + 3 * y_std,
    alpha=0.3,
    label="Confidence interval",
)
ax.legend(loc=9)
ax.set_xlabel("x")
ax.set_ylabel("y")
ax.set_xlim(-6, 6)
ax.set_ylim(-2.8, 3.5)
plt.show()
```

Total running time of the script: (0 minutes 0.198 seconds)

CHAPTER

FIVE

CHANGELOG

5.1 Version 1.6.1

September 02, 2021

New features

- IO routines for zmap files (#199)
- `write_asc_grid` got new keyword `no_data` (#199)

Changes

- now using a `pyproject.toml` file (#211)
- now using a single `main` branch in the repository (#212)
- Fixed typos (#188, #189)

Bug fixes

- `write_asc_grid` was to strict about dx (#197)

5.2 Version 1.6.0

April 04, 2021

New features

- added Classification Kriging (#165, #184)
- added wheels for Python 3.9 (#175)

Changes

- moved scikit-learn compat-class `Krige` to `pykrige.compat` (#165)
- dropped Python 3.5 support (#183)
- moved CI to GitHub-Actions (#175, #183)
- Fixed Typo in `02_kriging3D.py` example (#182)

5.3 Version 1.5.1

August 20, 2020

New features

- update Regression Kriging class to be compatible with all kriging features (#158)
- added option to enable/disable "exact values" to all kriging routines (#153)
- added option to use the pseudo-inverse in all kriging routines (#151)

Changes

- removed compat-layer for sklearn (#157)
- updated examples in documentation

5.4 Version 1.5.0

April 04, 2020

New features

- support for GSTools covariance models (#125)
- pre-build wheels for py35-py38 on Linux, Windows and MacOS (#142)
- GridSerachCV from the compat module sets iid=False by default (if present in sklearn) to be future prove (iid will be deprecated) (#144)

Changes

- dropped py2* and py<3.5 support (#142)
- installation now requires cython (#142)
- codebase was formatted with black (#144)
- internally use of scipys lapack/blas bindings (#142)
- PyKrige is now part of the GeoStat-Framework

5.5 Version 1.4.1

January 13, 2019

New features

- Added method to obtain variogram model points. PR#94 by Daniel Mejía Raigosa

Bug fixes

- Fixed OrdinaryKriging readme example. PR#107 by Harry Matchette-Downes
- Fixed kriging matrix not being calculated correctly for geographic coordinates. PR99 by Mike Rilee

5.6 Version 1.4.0

April 24, 2018

New features

- Regression kriging algotithm. PR #27 by Sudipta Basaks.
- Support for spherical coordinates. PR #23 by Malte Ziebarth
- Kriging parameter tuning with scikit-learn. PR #24 by Sudipta Basaks.
- Variogram model parameters can be specified using a list or a dict. Allows for directly feeding in the partial sill rather than the full sill. PR #47 by Benjamin Murphy.

Enhancements

- Improved memory usage in variogram calculations. PR #42 by Sudipta Basaks.
- Added benchmark scripts. PR #36 by Roman Yurchak
- Added an extensive example using the meusegrids dataset. PR #28 by kvanlombeek.

Bug fixes

- Statistics calculations in 3D kriging. PR #45 by Will Chang.
- Automatic variogram estimation robustified. PR #47 by Benjamin Murphy.

5.7 Version 1.3.1

December 10, 2016

- More robust setup for building Cython extensions

5.8 Version 1.3.0

October 23, 2015

- Added support for Python 3.
- Updated the setup script to handle problems with trying to build the Cython extensions. If the appropriate compiler hasn't been installed on Windows, then the extensions won't work (see [this discussion of using Cython extensions on Windows] for how to deal with this problem). The setup script now attempts to build the Cython extensions and automatically falls back to pure Python if the build fails. **NOTE that the Cython extensions currently are not set up to work in Python 3** (see [discussion in issue #10]), so they are not built when installing with Python 3. This will be changed in the future.
- [closed issue #2]: https://github.com/GeoStat-Framework/PyKrige/issues/2
- [this discussion of using Cython extensions on Windows]: https://github.com/cython/cython/wiki/CythonExtensionsOnWindows
- [discussion in issue #10]: https://github.com/GeoStat-Framework/PyKrige/issues/10

5.9 Version 1.2.0

August 1, 2015

- Updated the execution portion of each class to streamline processing and reduce redundancy in the code.
- Integrated kriging with a moving window for two-dimensional ordinary kriging. Thanks to Roman Yurchak for this addition. This can be very useful for working with very large datasets, as it limits the size of the kriging matrix system. However, note that this approach can also produce unexpected oddities if the spatial covariance of the data does not decay quickly or if the window is too small. (See Kitanidis 1997 for a discussion of potential problems in kriging with a moving window; also see [closed issue #2] for a brief note about important considerations when kriging with a moving window.)
- Integrated a Cython backend for two-dimensional ordinary kriging. Again, thanks to Roman Yurchak for this addition. Note that currently the Cython backend is only implemented for two-dimensional ordinary kriging; it is not implemented in any of the other kriging classes. (I'll gladly accept any pull requests to extend the Cython backend to the other classes.)
- Implemented two new generic drift capabilities that should allow for use of arbitrary user-designed drifts. These generic drifts are referred to as 'specified' and 'functional' in the code. They are available for both two-dimensional and three-dimensional universal kriging (see below). With the 'specified' drift capability, the user specifies the values of the drift term at every data point and every point at which the kriging system is to be evaluated. With the 'functional' drift capability, the user provides callable function(s) of the two or three spatial coordinates that define the drift term(s). The functions must only take the spatial coordinates as arguments. An arbitrary number of 'specified' or 'functional' drift terms may be used. See `UniversalKriging.__doc__` or `UniversalKriging3D.__doc__` for more information.
- Made a few changes to how the drift terms are implemented when the problem is anisotropic. The regional linear drift is applied in the adjusted coordinate frame. For the point logarithmic drift, the point coordinates are transformed into the adjusted coordinate frame and the drift values are calculated in the transformed frame. The external scalar drift values are extracted using the original (i.e., unadjusted) coordinates. Any functions that are used with the 'functional' drift capability are evaluated in the adjusted coordinate frame. Specified drift values are not adjusted as they are taken to be for the exact points provided.
- Added support for three-dimensional universal kriging. The previous three-dimensional kriging class has been renamed OrdinaryKriging3D within module ok3d, and the new class is called UniversalKriging3D within module uk3d. See `UniversalKriging3D.__doc__` for usage information. A regional linear drift ('regional_linear') is the only code-internal drift that is currently supported, but the 'specified' and 'functional' generic drift capabilities are also implemented here (see above). The regional linear drift is applied in all three spatial dimensions.

5.10 Version 1.1.0

May 25, 2015

- Added support for two different approaches to solving the entire kriging problem. One approach solves for the specified grid or set of points in a single vectorized operation; this method is default. The other approach loops through the specified points and solves the kriging system at each point. In both of these techniques, the kriging matrix is set up and inverted only once. In the vectorized approach, the rest of the kriging system (i.e., the RHS matrix) is set up as a single large array, and the whole system is solved with a single call to `numpy.dot()`. This approach is faster, but it can consume a lot of RAM for large datasets and/or large grids. In the looping approach, the rest of the kriging system (the RHS matrix) is set up at each point, and the kriging system at that point is solved with a call to `numpy.dot()`. This approach is slower, but it does not take as much memory. The approach can be specified by using the `backend` kwarg in the `execute()` method: `'vectorized'`

(default) for the vectorized approach, `'loop'` for the looping approach. Thanks to Roman Yurchak for these changes and optimizations.

- Added support for implementing custom variogram models. To do so, set `variogram_model` to `'custom'`. You must then also specify `variogram_parameters` as well as `variogram_function`, which must be a callable object that takes only two arguments, first a list of function parameters and then the distances at which to evaluate the variogram model. Note that currently the code will not automatically fit the custom variogram model to the data. You must provide the `variogram_parameters`, which will be passed to the callable `variogram_function` as the first argument.
- Modified anisotropy rotation so that coordinate system is rotated CCW by specified angle. The sense of rotation for 2D kriging is now the opposite of what it was before.
- Added support for 3D kriging. This is now available as class `Krige3D` in `pykrige.k3d`. The usage is essentially the same as with the two-dimensional kriging classes, except for a few extra arguments that must be passed during instantiation and when calling `Krige3D.execute()`. See `Krige3D.__doc__` for more information.

5.11 Version 1.0.3

February 15, 2015

- Fixed a problem with the tests that are performed to see if the kriging system is to be solved at a data point. (Tests are completed in order to determine whether to force the kriging solution to converge to the true data value.)
- Changed setup script.

5.12 Version 1.0

January 25, 2015

- Changed license to New BSD.
- Added support for point-specific and masked-grid kriging. Note that the arguments for the `OrdinaryKriging.execute()` and `UniversalKriging.execute()` methods have changed.
- Changed semivariogram binning procedure.
- Boosted execution speed by almost an order of magnitude.
- Fixed some problems with the external drift capabilities.
- Added more comprehensive testing script.
- Fixed slight problem with `read_asc_grid()` function in `kriging_tools`. Also made some code improvements to both the `write_asc_grid()` and `read_asc_grid()` functions in `kriging_tools`.

5.13 Version 0.2.0

November 23, 2014

- Consolidated backbone functions into a single module in order to reduce redundancy in the code. `OrdinaryKriging` and `UniversalKriging` classes now import and call the `core` module for the standard functions.
- Fixed a few glaring mistakes in the code.
- Added more documentation.

5.14 Version 0.1.2

October 27, 2014

- First complete release.

INDEX

Symbols

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