SciKit GStat Documentation

Release 0.2.5

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CHAPTER

ONE

WELCOME TO SCIKIT GSTAT'S DOCUMENTATION!

SciKit-Gstat is a scipy-styled analysis module for geostatistics. It includes two base classes *Variogram* and *DirectionalVariogram*. Both have a very similar interface and can compute experimental variograms and model variograms. The module makes use of a rich selection of semi-variance estimators and variogram model functions, while being extensible at the same time.

With version 0.2.4, the class *SpaceTimeVariogram* has been added. It computes space-time experimental variogram. However, space-time modeling is not implemented yet.

With version 0.25, the class `OrdinaryKriging` has been added. It is working and can be used. However, it is not documented, the arguments might still change, multiprocessing is not implemented and the krige algorithm is not yet very efficient.

Note: Scikit-gstat was rewritten in major parts. Most of the changes are internal, but the attributes and behaviour of the *Variogram* has also changed substantially. A detailed description of the new versions usage will follow. The last version of the old Variogram class, 0.1.8, is kept in the *version-0.1.8* branch on GitHub, but not developed any further. It is not compatible to the current version.

CHAPTER

TWO

HOW TO CITE

In case you use SciKit-GStat in other software or scientific publications, please reference this module. It is published and has a DOI. It can be cited as:

> Mälicke, Mirko, & Schneider, Helge David. (2018). mmaelicke/scikit-gstat: Geostatistical variogram toolbox (Version v0.2.2). Zenodo. http://doi.org/10.5281/zenodo.1345584

2.1 Installation

The package can be installed directly from the Python Package Index or GitHub. The version on GitHub might be more recent, as only stable versions are uploaded to the Python Package Index.

2.1.1 PyPI

The version from PyPI can directly be installed using pip

```
pip install scikit-gstat
```

2.1.2 GitHub

The most recent version from GitHub can be installed like:

```
git clone https://github.com/mmaelicke/scikit-gstat.git
cd scikit-gstat
pip install -r requirements.txt
python setup.py install
```

2.1.3 Note

Depending on you OS, you might run into problems installing all requirements in a clean Python environment. These problems are usually caused by the scipy and numba package, which might need to be compiled. From our experience, no problems should occur, when an environment manager like anaconda is used. Then, the requirements can be installed like:

```
conda install numpy, scipy, numba
```

2.2 Getting Started

2.2.1 Load the class and data

The main class of scikit-gstat is the Variogram. It can directly be imported from the module, called skgstat. The main class can easily be demonstrated on random data.

```
In [1]: from skgstat import Variogram

In [2]: import numpy as np

In [3]: import matplotlib.pyplot as plt

In [4]: plt.style.use('ggplot')

In [5]: np.random.seed(42)

In [6]: coordinates = np.random.gamma(20, 5, (50,2))

In [7]: np.random.seed(42)

In [8]: values = np.random.normal(20, 5, 50)
```

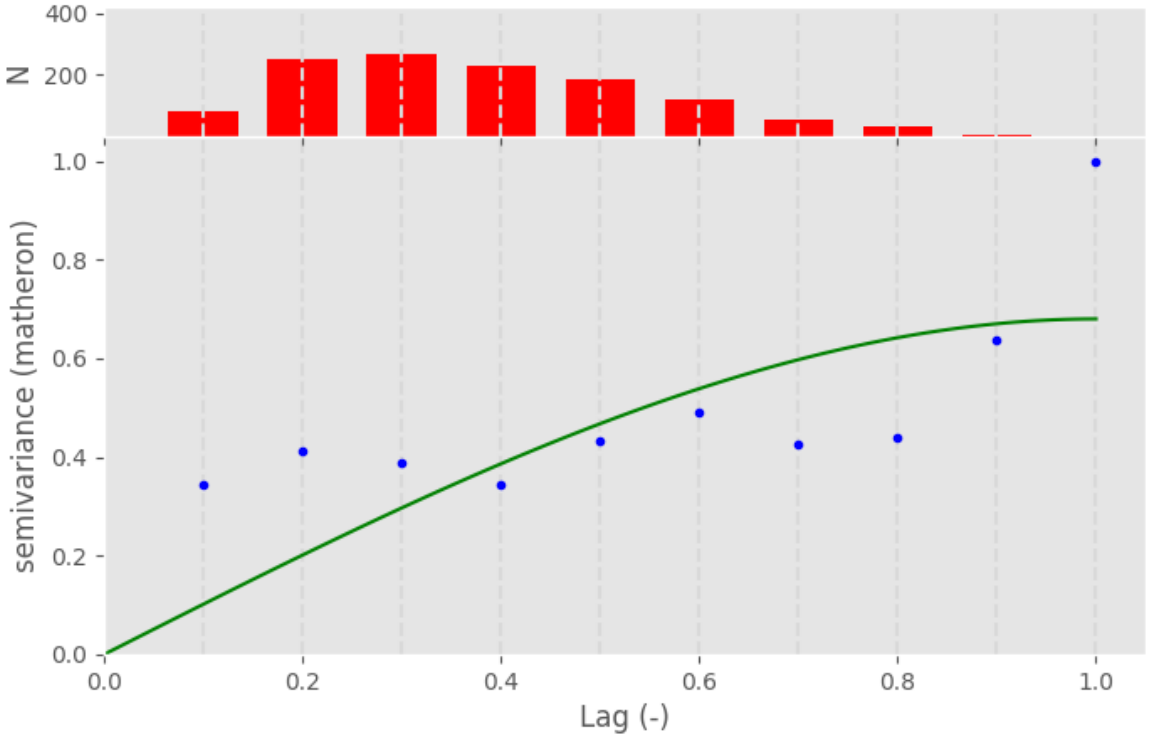
The Variogram needs at least an array of coordinates and an array of values on instantiation.

```
In [9]: V = Variogram(coordinates=coordinates, values=values)

In [10]: print(V)
spherical Variogram
--------------------
Estimator:         matheron

Effective Range:   10415.11

Sill:              1974.68

Nugget:            0.00
```

2.2.2 Plot

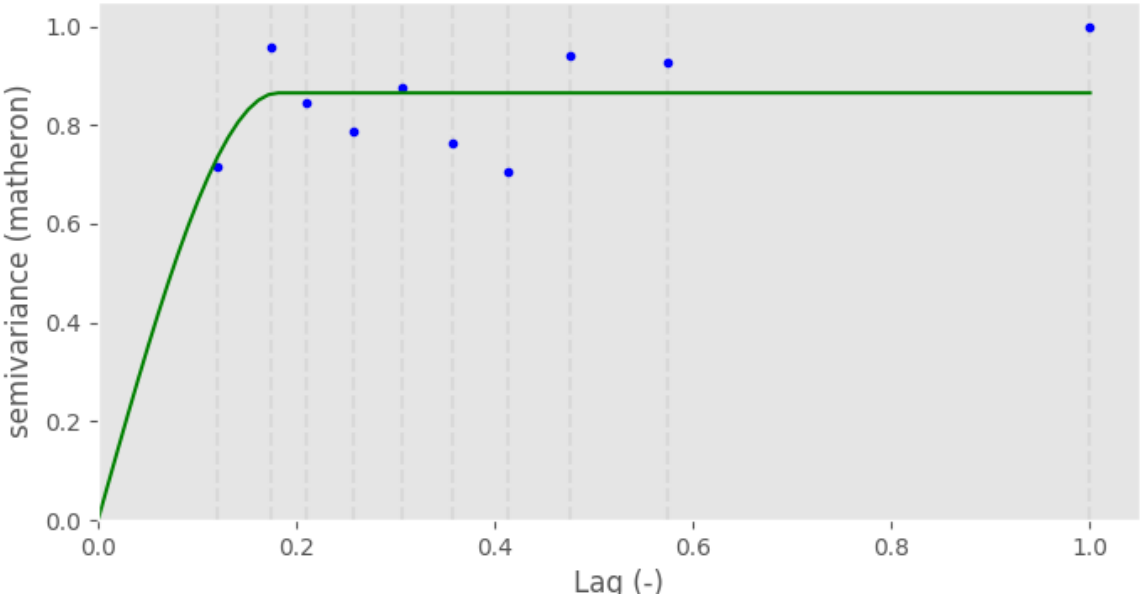
The Variogram class has its own plotting method.

```
In [11]: V.plot()
Out[11]: <Figure size 800x500 with 2 Axes>
```



With version 0.2, the histogram plot can also be disabled. This is most useful, when the binning method for the lag classes is changed from *'even'* step classes to *'uniform'* distribution in the lag classes.

```
In [12]: V.set_bin_func('uniform')

In [13]: V.plot(hist=False)
Out[13]: <Figure size 800x400 with 1 Axes>
```



2.3 User Guide

This user guide shall help you getting started with `scikit-gstat` package along with a more general introduction to variogram analysis.

2.3.1 Introduction

General

This user guide part of `scikit-gstat`'s documentation is meant to be an user guide to the functionality offered by the module along with a more general introduction to geostatistical concepts. The main use case is to hand this description to students learning geostatistics, whenever `scikit-gstat` is used. But before introducing variograms, the more general question what geostatistics actually are has to be answered.

Note: This user guide is meant to be an **introduction** to geostatistics. In case you are already familiar with the topic, you can skip this section.

What is geostatistics?

The basic idea of geostatistics is to describe and estimate spatial correlations in a set of point data. While the main tool, the variogram, is quite easy to implement and use, a lot of assumptions are underlying it. The typical application is geostatistics is an interpolation. Therefore, although using point data, a basic concept is to understand these point data as a sample of a (spatially) continuous variable that can be described as a random field rf, or to be more precise, a Gaussian random field in many cases. The most fundamental assumption in geostatistics is that any two values x_i and x_{i+h} are more similar, the smaller h is, which is a separating distance on the random field. In other words: *close observation points will show higher covariances than distant points*. In case this most fundamental conceptual

assumption does not hold for a specific variable, geostatistics will not be the correct tool to analyse and interpolate this variable.

One of the most easiest approaches to interpolate point data is to use IDW (inverse distance weighting). This technique is implemented in almost any GIS software. The fundamental conceptual model can be described as:

$$Z_u = \frac{\sum_i^N w_i * Z(i)}{N}$$

where Z_u is the value of rf at a non-observed location with N observations around it. These observations get weighted by the weight w_i, which can be calculated like:

$$w_i = \frac{1}{||\overrightarrow{ux_i}||}$$

where u is the not observed point and x_i is one of the sample points. Thus, $||\overrightarrow{ux_i}||$ is the 2-norm of the vector between the two points: the Euclidean distance in the coordinate space (which by no means has to be limited to the $\mathbb{R}^2$ case).

This basically describes a concept, where a value of the random field is estimated by a distance-weighted mean of the surrounding points. As close points shall have a higher impact, the inverse distance is used and thus the name of **inverse distance weighting**.

In the case of geostatistics this basic model still holds, but is extended. Instead of depending the weights exclusively on the separating distance, a weight will be derived from a variance over all values that are separated by a similar distance. This has the main advantage of incorporating the actual (co)variance found in the observations and basing the interpolation on this (co)variance, but comes at the cost of some strict assumptions about the statistical properties of the sample. Elaborating and assessing these assumptions is one of the main challenges of geostatistics.

Geostatistical Tools

Geostatistics is a wide field spanning a wide variety of disciplines, like geology, biology, hydrology or geomorphology. Each discipline defines their own set of tools, and apparently definitions, and progress is made until today. It is not the objective of `scikit-gstat` to be a comprehensive collection of all available tools. That would only be possible if professionals from each discipline contribute to the project. The objective is more to offer some common tools and simplify the process of geostatistical analysis and tool development thereby. However, you split geostatistics into three main fields, each of it with its own tools:

- **variography:** with the variogram being the main tool, the variography focuses on describing, visualizing and modelling covariance structures in space and time.
- **kriging:** is an interpolation method, that utilizes a variogram to find the estimate for weights as shown in the section above.
- **geostatistical simulation:** is aiming on generate random fields that fit a given set of observations or a pre-defined variogram.

Note: I am planning to implement common tools from all three fields. However, up to now, I am only focusing on variograms and no field generators or kriging procedures are available.

How to use this Guide

Write something about code examples and stuff

2.3.2 Variography

The variogram

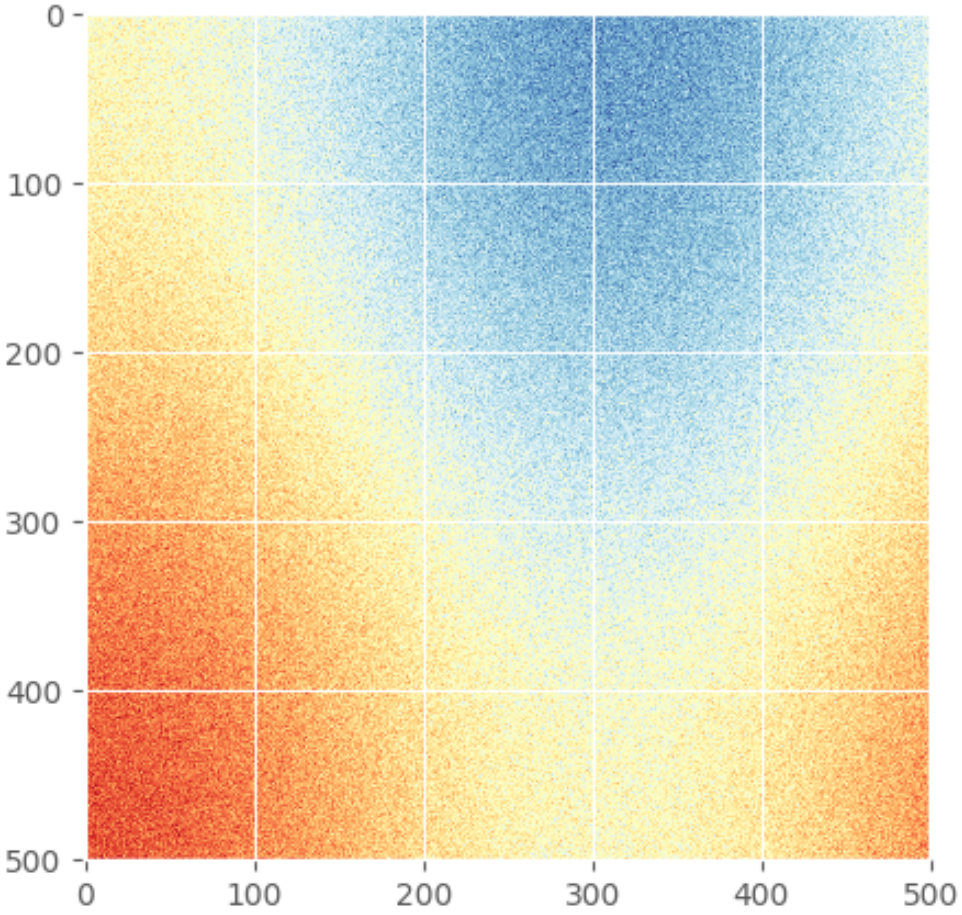
General

We start by constructing a random field and sample it. Without knowing about random field generators, an easy way to go is to stick two trigonometric functions together and add some noise. There should be clear spatial correlation apparent.

```
In [1]: import numpy as np

In [2]: import matplotlib.pyplot as plt

In [3]: plt.style.use('ggplot')
```

This field could look like

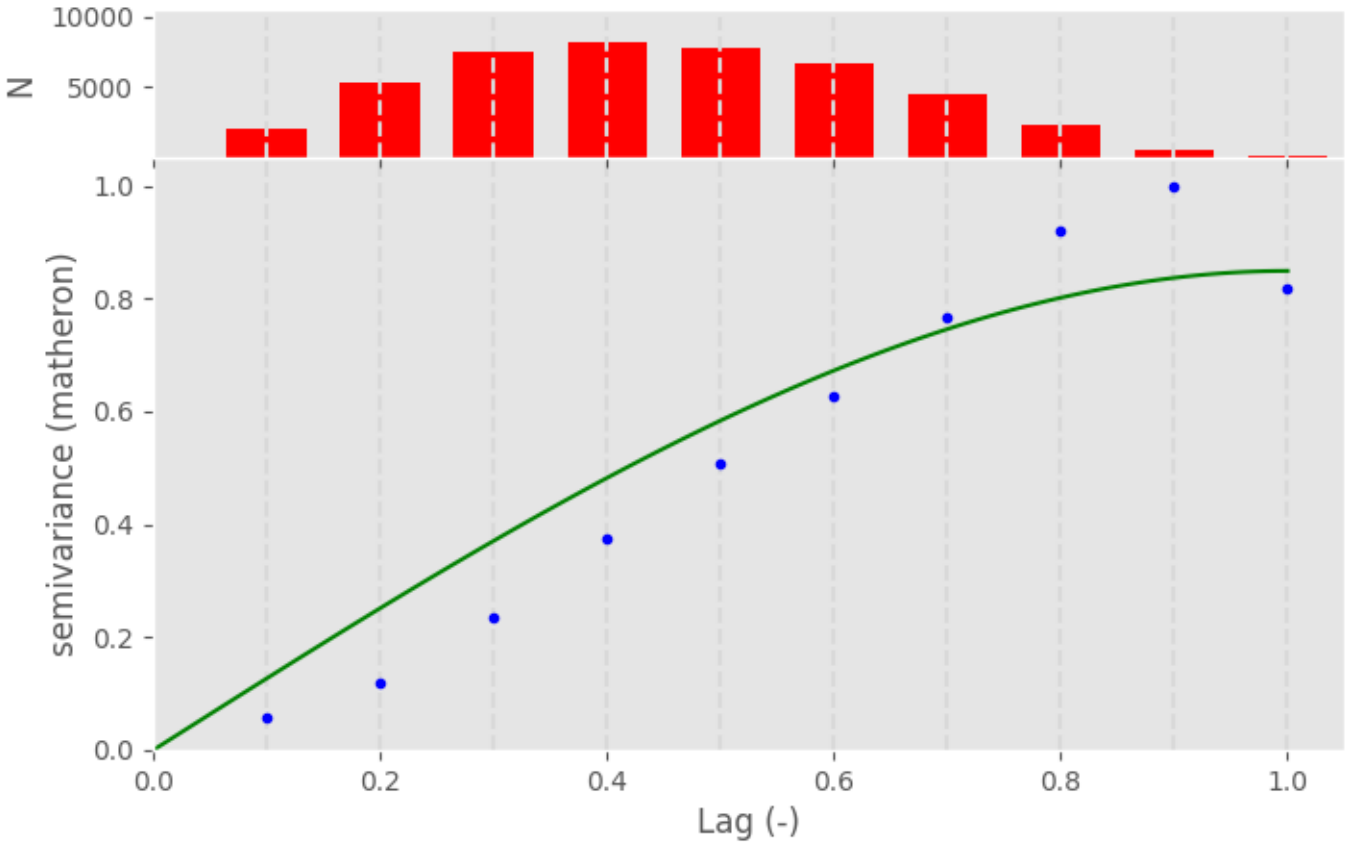
```
# apply the function to a meshgrid and add noise
In [4]: xx, yy = np.mgrid[0:0.5 * np.pi:500j, 0:0.8 * np.pi:500j]

In [5]: np.random.seed(42)

# generate a regular field
In [6]: _field = np.sin(xx)**2 + np.cos(yy)**2 + 10

# add noise
In [7]: np.random.seed(42)

In [8]: z = _field + np.random.normal(0, 0.15, (500,  500))

In [9]: plt.imshow(z, cmap='RdYlBu_r')
Out[9]: <matplotlib.image.AxesImage at 0x2ac9fa7b2080>
```



Using scikit-gstat

It's now easy and straightforward to calculate a variogram using `scikit-gstat`. We need to sample the field and pass the coordinates and value to the *`Variogram Class`*.

```
In [10]: from skgstat import Variogram

# random coordinates
In [11]: np.random.seed(42)

In [12]: coords = np.random.randint(0, 500, (300, 2))

In [13]: values = np.fromiter((z[c[0], c[1]] for c in coords), dtype=float)

In [14]: V = Variogram(coords, values)

In [15]: V.plot()
Out[15]: <Figure size 800x500 with 2 Axes>
```



From my personal point of view, there are three main issues with this approach:

- If one is not an geostatistics expert, one has no idea what he actually did and can see in the presented figure.
- The figure includes an spatial model, one has no idea if this model is suitable and fits the observations (wherever they are in the figure) sufficiently.
- Refer to the *__init__* method of the Variogram class. There are 10+ arguments that can be set optionally. The default values will most likely not fit your data and requirements.

Therefore one will have to understand how the *Variogram Class* works along with some basic knowledge about variography in oder to be able to properly use `scikit-gstat`.

However, what we can discuss from the figure, is what a variogram actually is At its core it relates a dependent variable to an independent variable and, in a second step, tries to describe this relationship with a statistical model. This model on its own describes some of the spatial properties of the random field and can further be utilized in an interpolation to select nearby points and weight them based on their statistical properties.

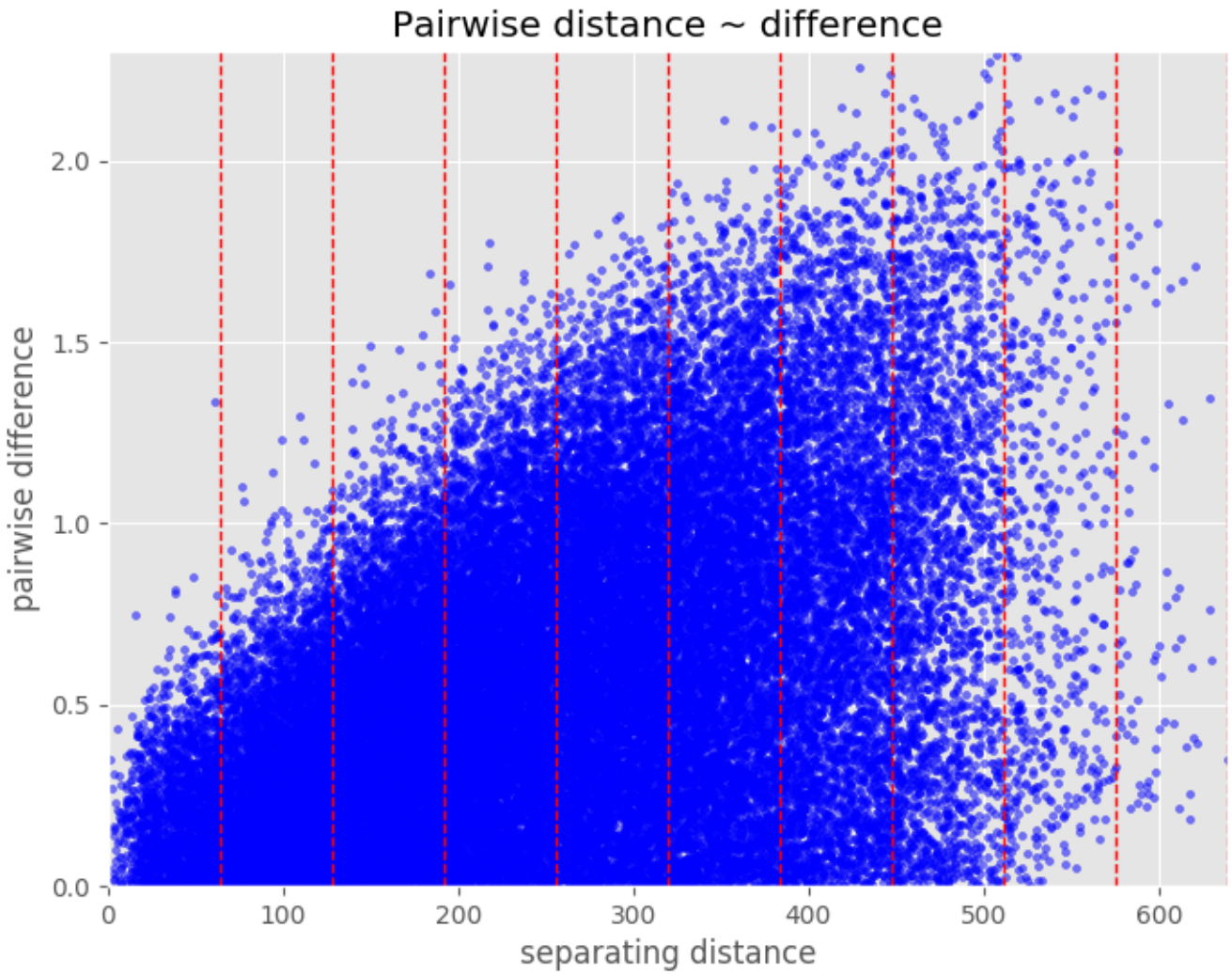
The variogram relates the separating distance between two observation points to a measure of variability of values at that given distance. Our expectation is that variance is increasing with distance, what can basically be seen in the presented figure.

Distance

Consider the variogram figure from above, with which an *independent* and *dependent* variable was introduced. In statistics it is common to use *dependent* variable as an alias for *target variable*, because its value is dependent on the state of the independent variable. In the case of a variogram, this is the metric of variance on the y-axis. The independent variable is a measure of (usually) Euclidean distance.

Consider observations taken in the environment, it is fairly unlikely to find two pairs of observations where the separating distance between the coordinates match exactly the same value. Therefore it is useful to group all point pairs at the same distance *lag* together into one group, or *bin*. Beside practicability, there is also another reason, why one would want to group point pairs at similar separating distances together into one bin. This becomes obvious, when one plots the difference in value over the distance for all point pair combinations that can be formed for a given sample. The *Variogram Class* has a function for that: *distance_difference_plot*:

```
In [16]: V.distance_difference_plot()
Out[16]: <Figure size 800x600 with 1 Axes>
```



While it is possible to see the increasing variability with increasing distance here quite nicely, it is not possible to guess

meaningful moments for the distributions within the bins. Last but not least, to derive a simple model as presented in the variogram figure above by the green line, we have to be able to compress all values at a given distance lag to one estimation of variance. This would not be possible from the the figure above.

Note: There are also procedures that can fit a model directly based on unbinned data. As none of these methods is implemented into `scikit-gstat`, they will not be discussed here. If you need them, you are more than welcome to implement them. Else you'll have to wait until I did that.

Binning the separating distances into distance lags is therefore a crucial and most important task in a variogram analysis. The final binning shall discretizise the distance lag at a meaningful resolution at the scale of interest while still holding enough members in the bin to make valid estimations. Often this is a trade-off relationship and one has to find a suitable compromise.

Before diving into binning, we have to understand how the *`Variogram Class`* handles distance data. The distance calculation can be controlled by the `dist_func` argument, which takes either a string or a function. The default value is *'euclidean'*. This value is directly passed down to the `pdist` as the *metric* argument.

`scikit-gstat` has two different methods for binning.

Note: This is not finished. Will continue whenever I can find some time.

Observation differences

Experimental variograms

When direction matters

What is 'direction'?

Space-time variography

2.4 Technical Notes

This chapter collects a number of technical advises for using scikit-gstat. These examples and information shall shall either explain the implementation or guide you to a correct usage of the packages. Not all features implemented make sense in every situation.

2.4.1 Fitting a theoretical model

General

The fit function of Variogram relies as of this writing on the `scipy.optimize.curve_fit()` function. That function can be used by ust passing a function and a set of x and y values and hoping for the best. However, this will not always yield the best parameters. Especially not for fitting a theoretical variogram function. There are a few assumptions and simplifications, that we can state in order to utilize the function in a more meaningful way.

Default fit

The example below shows the performance of the fully unconstrained fit, performed by the Levenberg-Marquardt algorithm. In scikit-gstat, this can be used by setting the *fit_method* parameter to *lm*. However, this is not recommended.

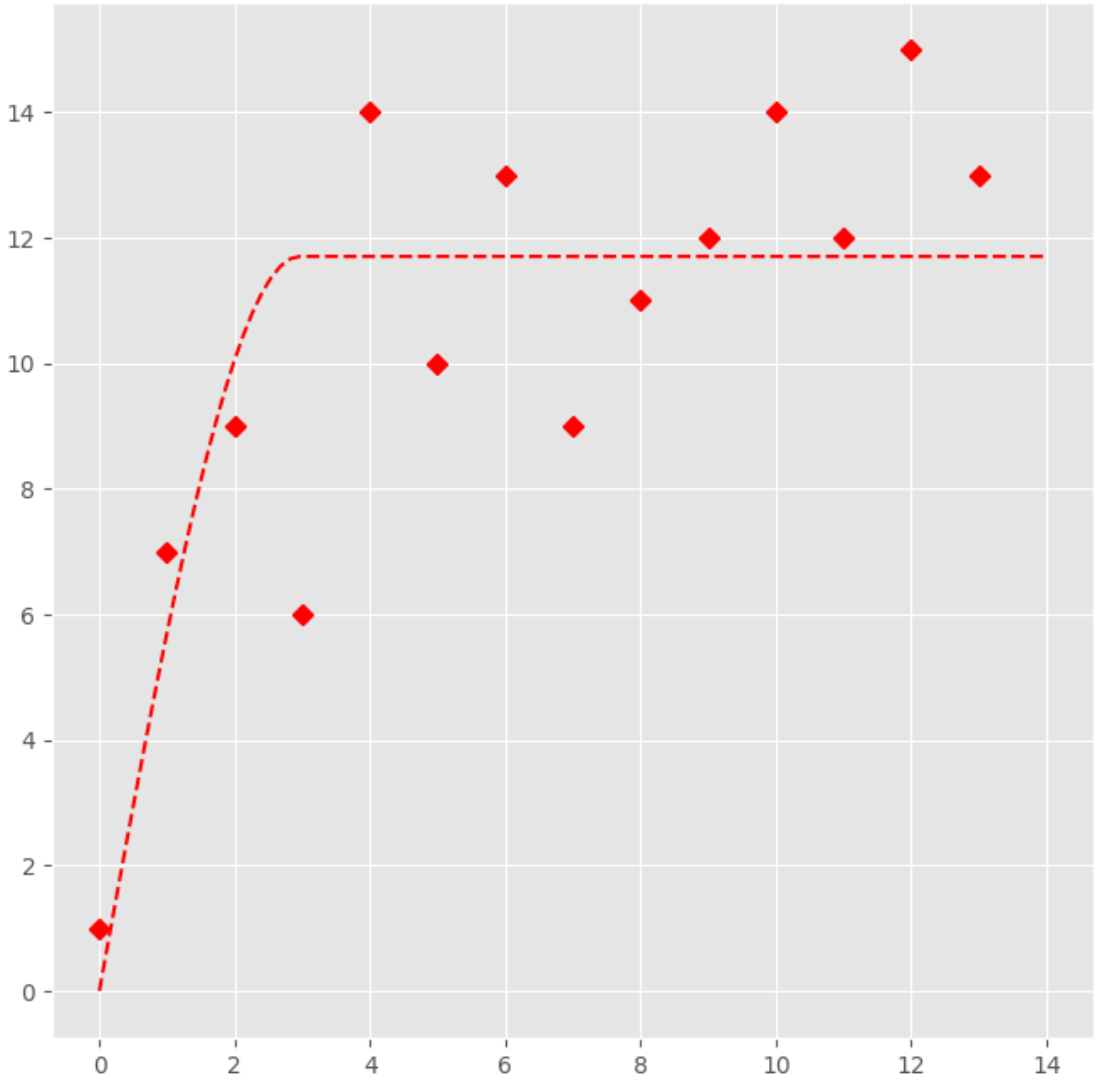
```
In [1]: from scipy.optimize import curve_fit

In [2]: import matplotlib.pyplot as plt

In [3]: plt.style.use('ggplot')

In [4]: import numpy as np

In [5]: from skgstat.models import spherical
```

The fit of a spherical model will be illustrated with some made-up data representing an experimental variogram:

```
In [6]: y = [1,7,9,6,14,10,13,9,11,12,14,12,15,13]

In [7]: x = list(range(len(y)))

In [8]: xi = np.linspace(0, len(y), 100)
```

As the *spherical* function is compiled using numba, we wrap the function in order to let `curve_fit` correctly infer the parameters. Then, fitting is a straightforward task.

```
In [9]: def f(h, a, b):
   ...:     return spherical(h, a, b)
   ...:

In [10]: cof_u, cov = curve_fit(f, x, y)

In [11]: yi = list(map(lambda x: spherical(x, *cof_u), xi))

In [12]: plt.plot(x, y, 'rD')
Out[12]: [<matplotlib.lines.Line2D at 0x2ac9fb2be0b8>]

In [13]: plt.plot(xi, yi, '--r')
\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\Out[13]: [<matplotlib.lines.
↪Line2D at 0x2ac9fb2be470>]
```



In fact this looks quite good. But Levenberg-Marquardt is an unconstrained fitting algorithm and it could likely fail on finding a parameter set. The `fit` method can therefore also run a box constrained fitting algorithm. It is the Trust Region Reflective algorithm, that will find parameters within a given range (box). It is set by the *fit_method='tfr'* parameter and also the default setting.

Constrained fit

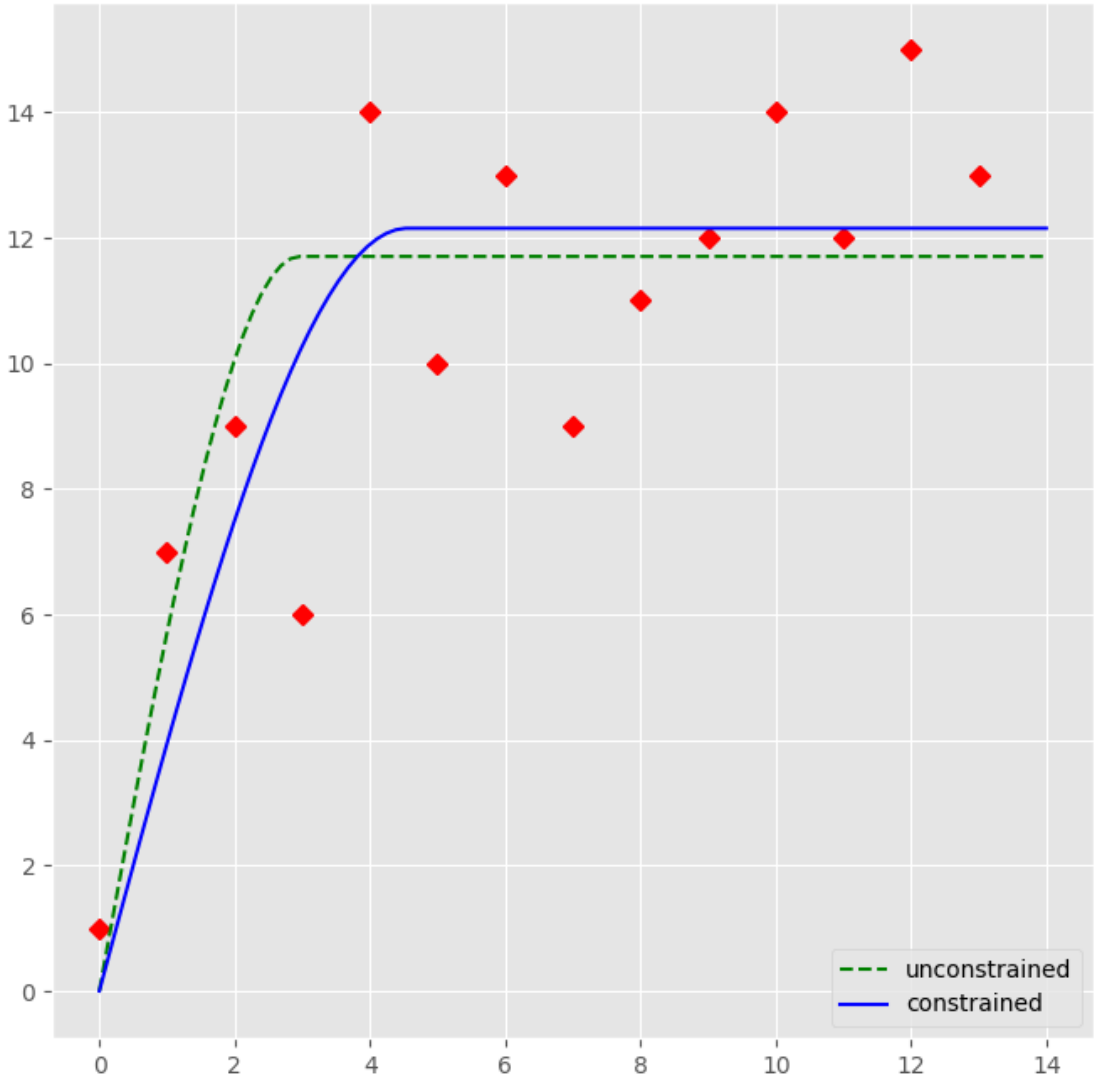
The constrained fitting case was chosen to be the default method in skgstat as the region can easily be specified. Furthermore it is possible to make a good guess on initial values. As we fit actual variogram parameters, namely the effective range, sill, nugget and in case of a stable or Matérn model an additional shape parameter, we know that these

parameters cannot be zero. The semi-variance is defined to be always positive. Thus the lower bound of the region will be zero in any case. The upper limit can easily be inferred from the experimental variogram. There are some simple rules, that all theoretical functions follow:

- the sill, nugget and their sum cannot be larger than the maximum empirical semi-variance
- the range cannot be larger than maxlag, or if maxlag is None the maximum value in the distances

The *Variogram* class will set the bounds to exactly these values as default behaviour. As an initial guess, it will use the mean value of semi-variances for the sill, the mean separating distance as range and 0 for the nugget. In the presented empirical variogram, difference between Levenberg-Marquardt and Trust Region Reflective is illustrated in the example below.

```
# default plot
In [14]: plt.plot(x, y, 'rD')
Out[14]: [<matplotlib.lines.Line2D at 0x2ac9fb244438>]

In [15]: plt.plot(xi, yi, '--g', label='unconstrained')
\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\Out[15]: [<matplotlib.lines.
↪Line2D at 0x2ac9fb244ac8>]

In [16]: cof, cov = curve_fit(f, x, y, p0=[3., 14.], bounds=(0, (np.max(x), np.
↪max(y))))

In [17]: yi = list(map(lambda x: spherical(x, *cof), xi))

In [18]: plt.plot(xi, yi, '-b', label='constrained')
Out[18]: [<matplotlib.lines.Line2D at 0x2ac9fb2df7f0>]

In [19]: plt.legend(loc='lower right')
\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\Out[19]: <matplotlib.legend.
↪Legend at 0x2ac9fb2df278>
```



The constrained fit, represented by the solid blue line is significantly different from the unconstrained fit (dashed, green line). The fit is overall better as a quick RMSE calculation shows:

```
In [20]: rmse_u = np.sqrt(np.sum([(spherical(_, *cof_u) - _)**2 for _ in x]))

In [21]: rmse_c = np.sqrt(np.sum([(spherical(_, *cof) - _)**2 for _ in x]))

In [22]: print('RMSE unconstrained: %.2f' % rmse_u)
RMSE unconstrained: 18.65

In [23]: print('RMSE constrained:   %.2f' % rmse_c)
\\\\\\\\\\\\\\\\\\\\\\\\\\\\RMSE constrained:   17.42
```

The last note about fitting a theoretical function, is that both methods assume all lag classes to be equally important for the fit. In the specific case of a variogram this is not true.

Distance weighted fit

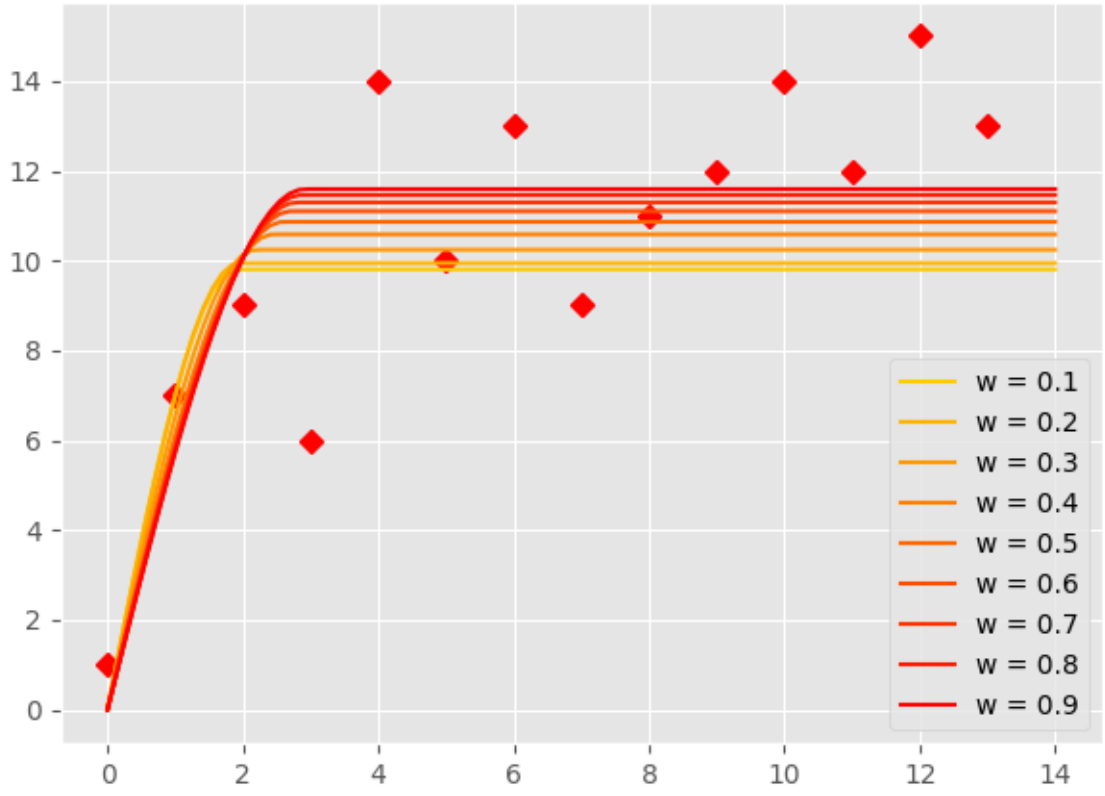
While the standard Levenberg-Marquardt and Trust Region Reflective algorithms are both based on the idea of least squares, they assume all observations to be equally important. In the specific case of a theoretical variogram function, this is not the case. The variogram describes a dependency of covariance in value on the separation distances of the observations. This model already implies that the dependency is stronger on small distances. Considering a kriging interpolation as the main application of the variogram model, points on close distances will get higher weights for the interpolated value of an unobserved location. The weight on large distances will be neglected anyway. Hence, a good fit on small separating distances is way more important. The `curve_fit` function does not have an option for weighting the squares of specific observations. At least it does not call it 'weights'. In terms of scipy, you can define a 'sigma', which is the uncertainty of the respective point. The uncertainty σ influences the least squares calculation as described by the equation:

$$\chi_{sq} = \sum \left(\frac{r}{\sigma}\right)^2$$

That means, the larger σ is, the *less* weight it will receive. That also means, we can almost ignore points, by assigning a ridiculous high σ to them. The following example should illustrate the effect. This time, the first 7 points will be weighted by a weight $\sigma = [0.1, 0.2, \ldots 0.9]$ and the remaining points will receive a $\sigma = 1$. In the case of $\sigma = 0.1$, this would change the least squares cost function to:

$$\chi_{sq;x_{1:7}} = \sum (10r)^2$$

```
In [24]: cm = plt.get_cmap('autumn_r')

In [25]: sigma = np.ones(len(x))

In [26]: fig, ax = plt.subplots(1, 1, figsize=(7, 5))

In [27]: ax.plot(x, y, 'rD')
Out[27]: [<matplotlib.lines.Line2D at 0x2ac9fb2f9c88>]

In [28]: for w in np.arange(0.1, 1., 0.1):
   ....:     s = sigma.copy()
   ....:     s[:6] *= w
   ....:     cof, cov = curve_fit(f, x, y, sigma=s)
   ....:     yi = list(map(lambda x: spherical(x, *cof), xi))
   ....:     ax.plot(xi, yi, linestyle='-', color=cm(w + 0.1), label='w = %.1f' % w)
   ....:

In [29]: ax.legend(loc='lower right')
Out[29]: <matplotlib.legend.Legend at 0x2ac9fb30ff28>
```



In the figure above, you can see how the last points get more and more ignored by the fitting. A smaller w value means more weight on the first 7 points. The more yellow lines have a smaller sill and range.

The *Variogram* class accepts lists like sigma from the code example above as *Variogram.fit_sigma* property. This way, the example from above could be implemented. However, *Variogram.fit_sigma* can also apply a function of distance to the lag classes to derive the σ values. There are several predefined functions. These are:

- sigma='linear': The residuals get weighted by the lag distance normalized to the maximum lag distance, denoted as w_n
- sigma='exp': The residuals get weighted by the function: $w = e^{1/w_n}$
- sigma='sqrt': The residuals get weighted by the function: $w = \sqrt{(w_n)}$
- sigma='sq': The residuals get weighted by the function: $w = w_n^2$

The example below illustrates their effect on the sample experimental variograms used so far.

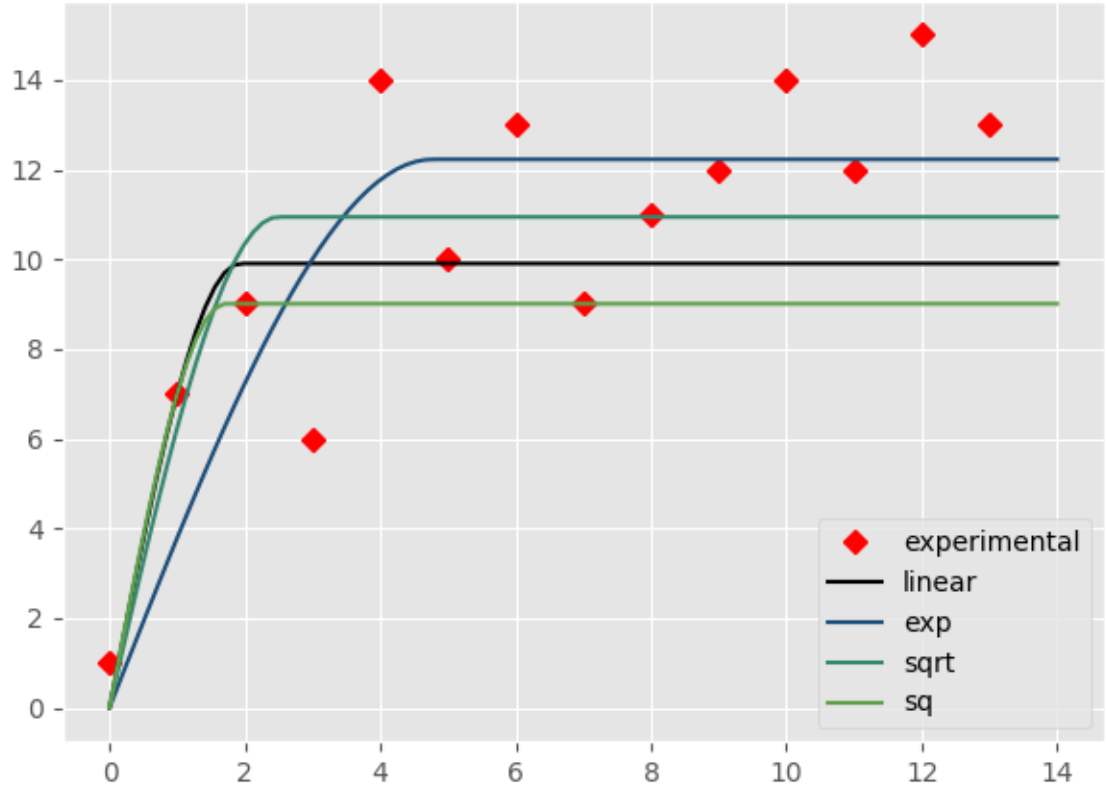
```
In [30]: cm = plt.get_cmap('gist_earth')

# increase the distance by one, to aviod zeros
In [31]: X = np.asarray([(_ + 1) for _ in x])

In [32]: s1 = X / np.max(X)

In [33]: s2 = np.exp(1. / X)
```

(continues on next page)

(continued from previous page)

```
In [34]: s3 = np.sqrt(s1)

In [35]: s4 = np.power(s1, 2)

In [36]: s = (s1, s2, s3, s4)

In [37]: labels = ('linear', 'exp', 'sqrt', 'sq')
```

```
In [38]: plt.plot(x, y, 'rD', label='experimental')
Out[38]: [<matplotlib.lines.Line2D at 0x2ac9fa88a2e8>]

In [39]: for i in range(4):
   ....:     cof, cov = curve_fit(f, x, y, sigma=s[i], p0=(6.,14.), bounds=(0,(14,
↪14)))
   ....:     yi = list(map(lambda x: spherical(x, *cof), xi))
   ....:     plt.plot(xi, yi, linestyle='-', color=cm((i/6)), label=labels[i])
   ....:

In [40]: plt.legend(loc='lower right')
Out[40]: <matplotlib.legend.Legend at 0x2ac9fa85e320>
```



That's it.

2.4.2 Directional Variograms

General

With version 0.2.2, directional variograms have been introduced. A directional variogram is a variogram where point pairs are only included into the semivariance calculation if they fulfill a specified spatial relation. This relation is expressed as a *search area* that identifies all *directional* points for a given specific point. SciKit-GStat refers to this point as *poi* (point of interest). The implementation is done by the *DirectionalVariogram* class.

Understanding Search Area

Note: The *DirectionalVariogram* is in general capable of handling n-dimensional coordinates. The application of directional dependency is, however, only applied to the first two dimensions.

Understanding the search area of a directional is vital for using the *DirectionalVariogram* class. The search area is controlled by the `directional_model` property which determines the shape of the search area. The extend and orientation of this area is controlled by the parameters:

- *azimuth*
- *tolerance*
- *bandwidth*

As of this writing, SciKit-GStat supports three different search area shapes:

- *triangle* (*default*)
- *circle*
- *compass*

Additionally, the shape generation is controlled by the *tolerance* parameter (*triangle*, *compass*) and *bandwidth* parameter (*triangle*, *circle*). The *azimuth* is used to rotate the search area into a desired direction. An azimuth of 0° is heading East of the coordinate plane. Positive values for azimuth rotate the search area clockwise, negative values counter-clockwise. The *tolerance* specifies how far the angle (against 'x-axis') between two points can be off the azimuth to be still considered as a directional point pair. Based on this definition, two points at a larger distance would generally be allowed to differ more from azimuth in terms of coordinate distance. Therefore the *bandwidth* defines a maximum coordinate distance, a point can have from the azimuth line. The difference between the *triangle* and the *compass* search area is that the triangle uses the bandwidth and the compass does not.

The *DirectionalVariogram* has a function to plot the current search area. As the search area is specific to the current poi, it has to be defined as the index of the coordinate to be used. The method is called *search_area*. Using random coordinates, the search area shapes are presented below.

```
In [1]: from skgstat import DirectionalVariogram

In [2]: import numpy as np

In [3]: import matplotlib.pyplot as plt

In [4]: plt.style.use('ggplot')

In [5]: np.random.seed(42)
```

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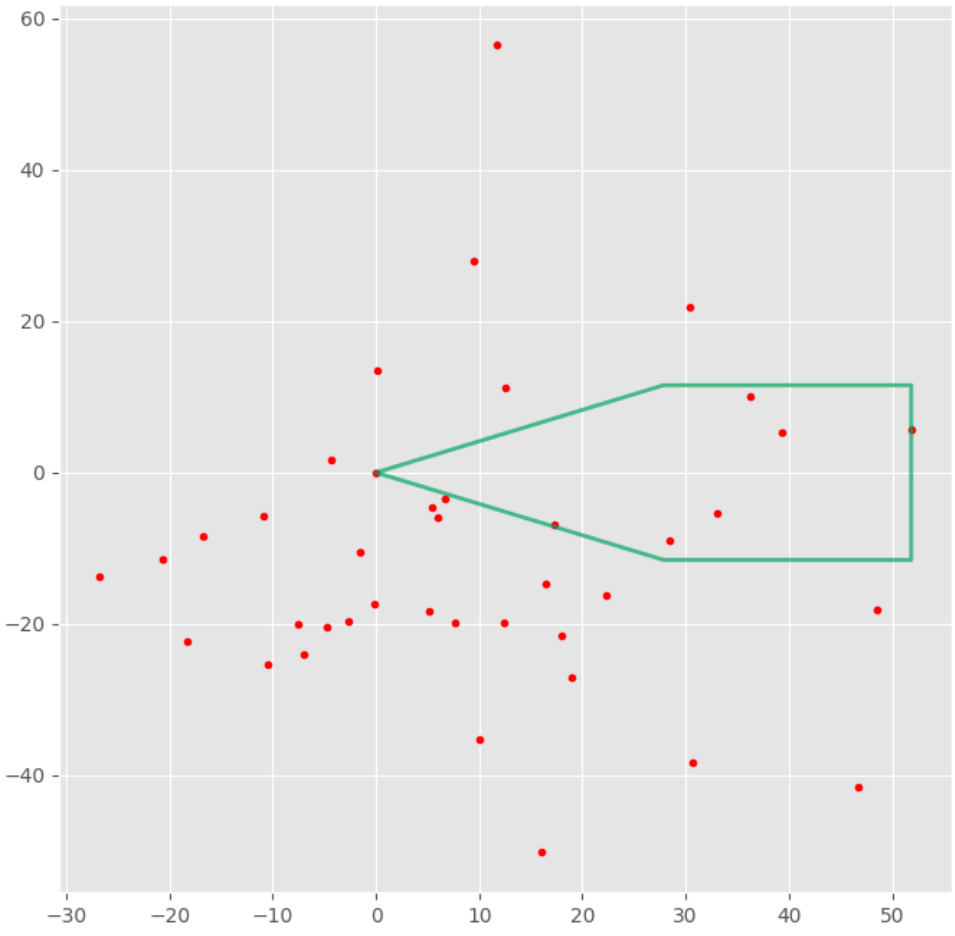
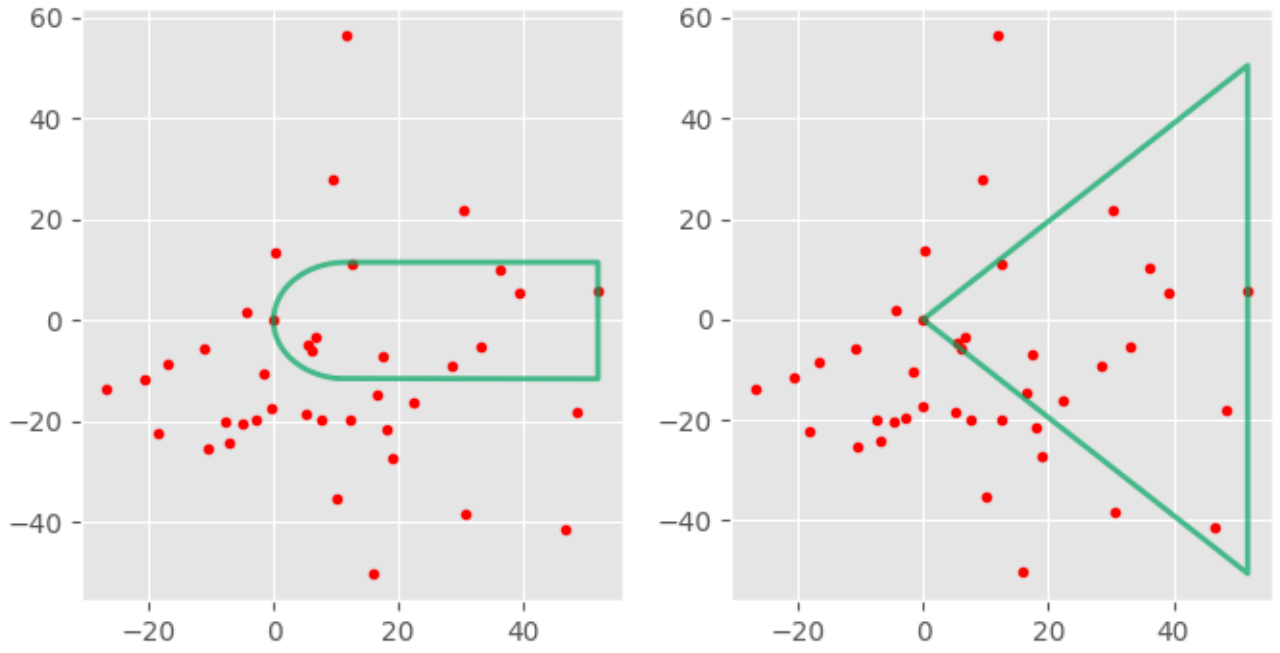
```
In [6]: coords = np.random.gamma(15, 6, (40, 2))

In [7]: np.random.seed(42)

In [8]: vals = np.random.normal(5,1, 40)

In [9]: DV = DirectionalVariogram(coords, vals,
   ...:     azimuth=0,
   ...:     tolerance=45,
   ...:     directional_model='triangle')
   ...:

In [10]: DV.search_area(poi=3)
Out[10]: <Figure size 800x800 with 1 Axes>
```



The model can easily be changed, using the *set_directional_model* function:

```
In [11]: fig, axes = plt.subplots(1, 2, figsize=(8, 4))

In [12]: DV.set_directional_model('circle')

In [13]: DV.search_area(poi=3, ax=axes[0])
Out[13]: <Figure size 800x400 with 2 Axes>

In [14]: DV.set_directional_model('compass')

In [15]: DV.search_area(poi=3, ax=axes[1])
Out[15]: <Figure size 800x400 with 2 Axes>

In [16]: fig.show()
```



Local Reference System

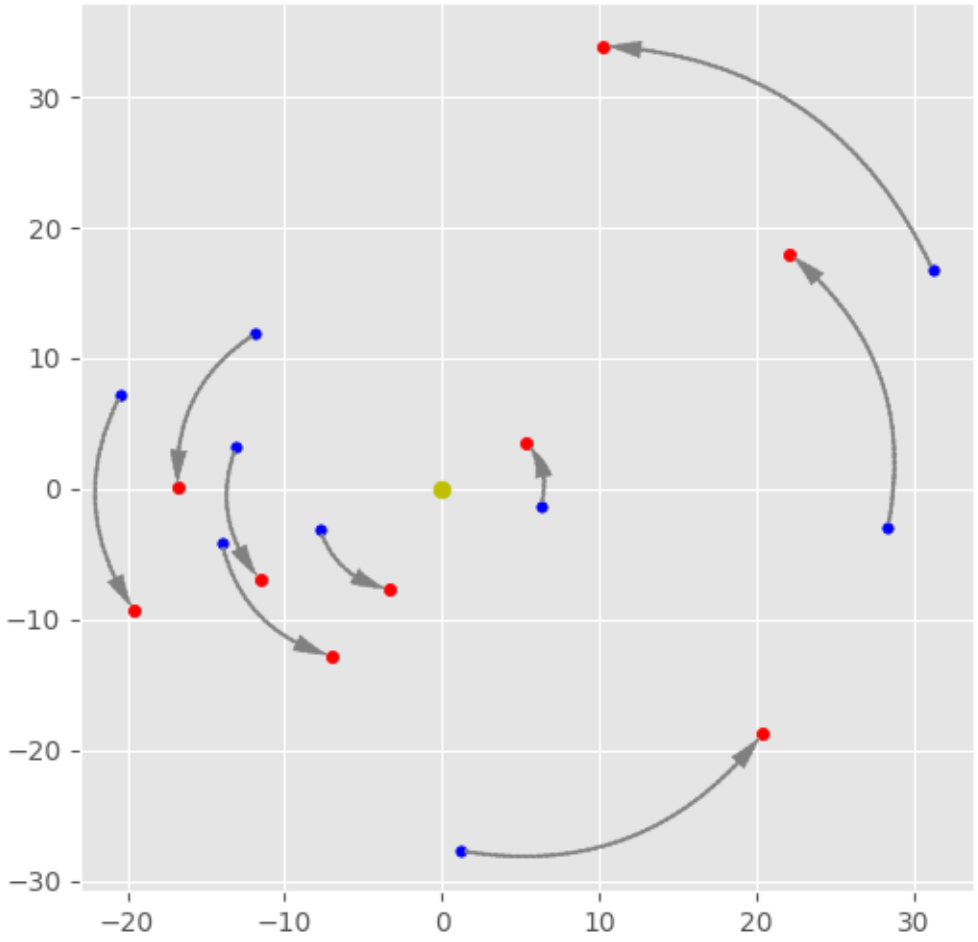
In order to apply different search area shapes and rotate them considering the given azimuth, a few preprocessing steps are necessary. This can lead to some calculation overhead, as in the case of a *compass* model. The selection of point pairs being directional is implemented by transforming the coordinates into a local reference system iteratively for each coordinate. For multidimensional coordinates, only the first two dimensions are used. They are shifted to make the current point of interest the origin of the local reference system. Then all other points are rotated until the azimuth overlays the local x-axis. This makes the definition of different shapes way easier. In this local system, the bandwidth can easily be applied to the transformed y-axis. The *set_directional_model* can also set a custom function as search area shape, that accepts the current local reference system and returns the search area for the given poi. The search area has to be returned as a shapely Polygon. Unfortunately, the *tolerance* and *bandwidth* parameter are not passed yet.

Note: For the next release, it is planned to pass all necessary parameters to the directional model function. This

should greatly improve the definition of custom shapes. Until the implementation, the parameters have to be injected directly.

The following example will illustrate the rotation of the local reference system.

```
In [17]: from matplotlib.patches import FancyArrowPatch as arrow

In [18]: np.random.seed(42)

In [19]: c = np.random.gamma(10, 6, (9, 2))

In [20]: mid = np.array([[np.mean(c[:,0]), np.mean(c[:,1])]])

In [21]: coords = np.append(mid, c, axis=0) - mid

In [22]: DV = DirectionalVariogram(coords, vals[:10],
   ....:     azimuth=45, tolerance=45)
   ....:

In [23]: loc = DV.local_reference_system(poi=0)

In [24]: fig, ax = plt.subplots(1, 1, figsize=(6, 6))

In [25]: ax.scatter(coords[:,0], coords[:,1], 15, c='b')
Out[25]: <matplotlib.collections.PathCollection at 0x2ac9faa956d8>

In [26]: ax.scatter(loc[:,0], loc[:,1], 20, c='r')
\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\Out[26]:
↪<matplotlib.collections.PathCollection at 0x2ac9fada83c8>

In [27]: ax.scatter([0], [0], 40, c='y')
\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
↪<matplotlib.collections.PathCollection at 0x2ac9fad9a940>

In [28]: for u,v in zip(coords[1:], loc[1:]):
   ....:     arrowstyle="Simple,head_width=6,head_length=12,tail_width=1"
   ....:     a = arrow(u, v,  color='grey', linestyle='--',
   ....:         connectionstyle="arc3, rad=.3", arrowstyle=arrowstyle)
   ....:     ax.add_patch(a)
   ....:

In [29]: fig.show()
```



After moving and shifting, any type of Geometry could be generated and passed as the search area.

```
In [30]: from shapely.geometry import Polygon

In [31]: def M(loc):
   ....:     xmax = np.max(loc[:,0])
   ....:     ymax = np.max(loc[:,1])
   ....:     return Polygon([
   ....:         (0, 0),
   ....:         (0, ymax * 0.6),
   ....:         (0.05*xmax, ymax * 0.6),
   ....:         (xmax * 0.3, ymax * 0.3),
   ....:         (0.55 * xmax, 0.6 * ymax),
   ....:         (0.6 * xmax, 0.6 * ymax),
   ....:         (0.6 * xmax, 0),
   ....:         (0.55 * xmax, 0),
   ....:         (0.55 * xmax, 0.55 * ymax),
   ....:         (xmax * 0.325, ymax * 0.275),
```

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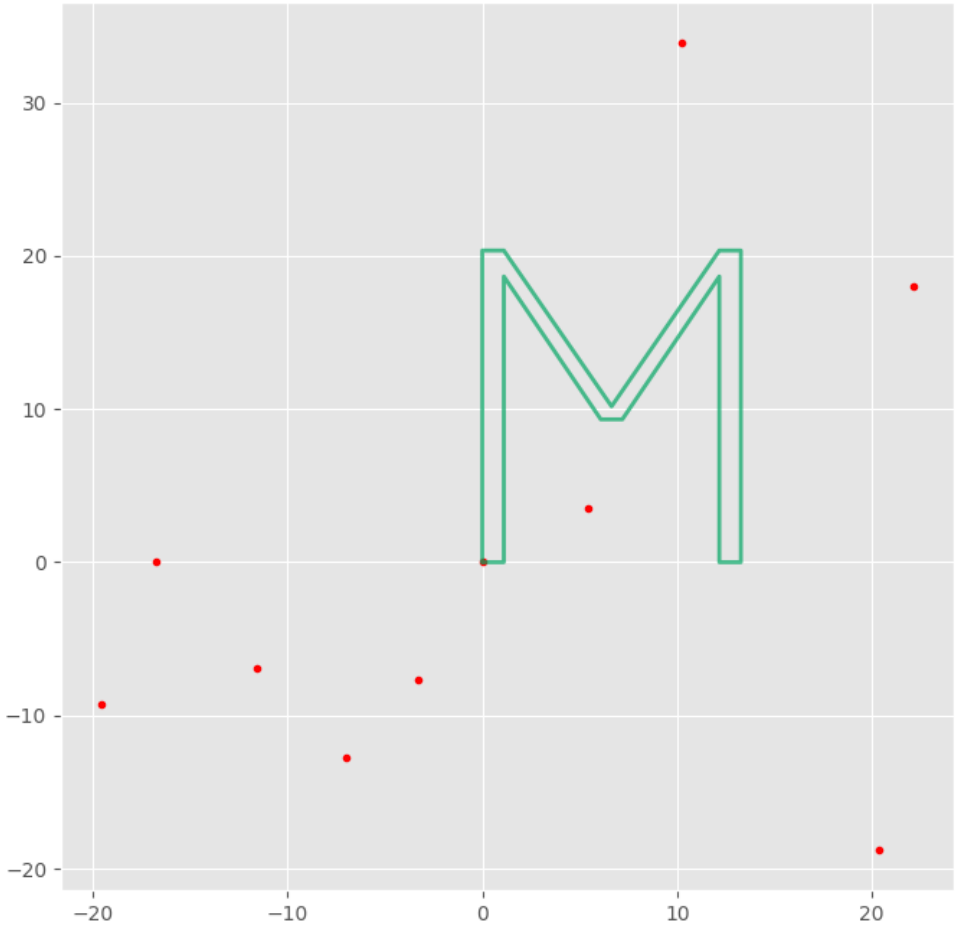
```
   ....:           (xmax * 0.275, ymax * 0.275),
   ....:           (0.05 * xmax, 0.55 * ymax),
   ....:           (0.05 * xmax, 0),
   ....:           (0, 0)
   ....:       ])
   ....:

In [32]: DV.set_directional_model(M)

In [33]: DV.search_area(poi=0)
Out[33]: <Figure size 800x800 with 1 Axes>
```



Directional variograms

In principle, the *DirectionalVariogram* can be used just like the *Variogram* base class. In fact *DirectionalVariogram* inherits most of the behaviour. All the functionality described in the previous sections

is added to the basic *Variogram*. All other methods and attributes can be used in the same way.

Warning: In order to implement the directional dependency, some methods have been rewritten in *DirectionalVariogram*. Thus the following methods do **not** show the same behaviour:

- DirectionalVariogram.bins
- DirectionalVariogram._calc_groups

2.5 Code Reference

2.5.1 Variogram Class

class skgstat.**Variogram**(*coordinates=None*, *values=None*, *estimator='matheron'*, *model='spherical'*, *dist_func='euclidean'*, *bin_func='even'*, *normalize=True*, *fit_method='trf'*, *fit_sigma=None*, *use_nugget=False*, *maxlag=None*, *n_lags=10*, *verbose=False*, *harmonize=False*)

Variogram Class

Calculates a variogram of the separating distances in the given coordinates and relates them to one of the semi-variance measures of the given dependent values.

__init__(*coordinates=None*, *values=None*, *estimator='matheron'*, *model='spherical'*, *dist_func='euclidean'*, *bin_func='even'*, *normalize=True*, *fit_method='trf'*, *fit_sigma=None*, *use_nugget=False*, *maxlag=None*, *n_lags=10*, *verbose=False*, *harmonize=False*)

Variogram Class

Note: The directional variogram estimation is not re-implemented yet. Therefore the parameters is-directional, azimuth and tolerance will be ignored at the moment and can be subject to changes.

Parameters

- **coordinates** (*numpy.ndarray*) – Array of shape (m, n). Will be used as m observation points of n-dimensions. This variogram can be calculated on 1 - n dimensional coordinates. In case a 1-dimensional array is passed, a second array of same length containing only zeros will be stacked to the passed one.
- **values** (*numpy.ndarray*) – Array of values observed at the given coordinates. The length of the values array has to match the m dimension of the coordinates array. Will be used to calculate the dependent variable of the variogram.
- **estimator** (*str, callable*) – String identifying the semi-variance estimator to be used. Defaults to the Matheron estimator. Possible values are:
  - matheron [Matheron, default]
  - cressie [Cressie-Hawkins]
  - dowd [Dowd-Estimator]
  - genton [Genton]
  - minmax [MinMax Scaler]
  - entropy [Shannon Entropy]

If a callable is passed, it has to accept an array of absoulte differences, aligned to the 1D distance matrix (flattened upper triangle) and return a scalar, that converges towards small values for similarity (high covariance).

- **model** (*str*) – String identifying the theoretical variogram function to be used to describe the experimental variogram. Can be one of:
  - spherical [Spherical, default]
  - exponential [Exponential]
  - gaussian [Gaussian]
  - cubic [Cubic]
  - stable [Stable model]
  - matern [Matérn model]
  - nugget [nugget effect variogram]
- **dist_func** (*str*) – String identifying the distance function. Defaults to 'euclidean'. Can be any metric accepted by scipy.spatial.distance.pdist. Additional parameters are not (yet) passed through to pdist. These are accepted by pdist for some of the metrics. In these cases the default values are used.
- **bin_func** (*str*) – String identifying the binning function used to find lag class edges. At the moment there are two possible values: 'even' (default) or 'uniform'. Even will find n_lags bins of same width in the interval [0,maxlag[. 'uniform' will identfy n_lags bins on the same interval, but with varying edges so that all bins count the same amount of observations.
- **normalize** (*bool*) – Defaults to False. If True, the independent and dependent variable will be normalized to the range [0,1].
- **fit_method** (*str*) – String identifying the method to be used for fitting the theoretical variogram function to the experimental. More info is given in the Variogram.fit docs. Can be one of:
  - 'lm': Levenberg-Marquardt algorithm for unconstrained problems. This is the faster algorithm, yet is the fitting of a variogram not unconstrianed.
  - 'trf': Trust Region Reflective function for non-linear constrained problems. The class will set the boundaries itself. This is the default function.
- **fit_sigma** (*numpy.ndarray, str*) – Defaults to None. The sigma is used as measure of uncertainty during variogram fit. If fit_sigma is an array, it has to hold n_lags elements, giving the uncertainty for all lags classes. If fit_sigma is None (default), it will give no weight to any lag. Higher values indicate higher uncertainty and will lower the influcence of the corresponding lag class for the fit. If fit_sigma is a string, a pre-defined function of separating distance will be used to fill the array. Can be one of:
  - 'linear': Linear loss with distance. Small bins will have higher impact.
  - 'exp': The weights decrease by a e-function of distance
  - 'sqrt': The weights decrease by the squareroot of distance
  - 'sq': The weights decrease by the squared distance.

  More info is given in the Variogram.fit_sigma documentation.

- **use_nugget** (*bool*) – Defaults to False. If True, a nugget effet will be added to all Variogram.models as a third (or fourth) fitting parameter. A nugget is essentially the y-axis interception of the theoretical variogram function.
- **maxlag** (*float, str*) – Can specify the maximum lag distance directly by giving a value larger than 1. The binning function will not find any lag class with an edge larger than maxlag. If 0 < maxlag < 1, then maxlag is relative and maxlag * max(Variogram.distance) will be used. In case maxlag is a string it has to be one of 'median', 'mean'. Then the median or mean of all Variogram.distance will be used. Note maxlag=0.5 will use half the maximum separating distance, this is not the same as 'median', which is the median of all separating distances
- **n_lags** (*int*) – Specify the number of lag classes to be defined by the binning function.
- **verbose** (*bool*) – Set the Verbosity of the class. Not Implemented yet.
- **harmonize** (*bool*) – this kind of works so far, but will be rewritten (and documented)

NS

Nash Sutcliffe efficiency of the fitted Variogram

Returns

bin_func

Binning function

Returns an instance of the function used for binning the separating distances into the given amount of bins. Both functions use the same signature of func(distances, n, maxlag).

The setter of this property utilizes the Variogram.set_bin_func to set a new function.

Returns **binning_function**

Return type function

See also:

Variogram.set_bin_func

clone()

Deep copy of self

Return a deep copy of self.

Returns

Return type *Variogram*

compiled_model

Compiled theoretical variogram model

Compile the model using the actual fitting parameters to return a function implementing them.

The compiled_model will be removed in version 0.3. Use the *Variogram.fitted_model* property instead. It is works in the same way, but is significantly faster

Returns

Return type callable

coordinates

Coordinates property

Array of observation locations the variogram is build for. This property has no setter. If you want to change the coordinates, use a new Variogram instance.

Returns coordinates

Return type numpy.array

data(*n=100*, *force=False*)
Theoretical variogram function

Calculate the experimental variogram and apply the binning. On success, the variogram model will be fitted and applied to n lag values. Returns the lags and the calculated semi-variance values. If force is True, a clean preprocessing and fitting run will be executed.

Parameters

- **n** (*integer*) – length of the lags array to be used for fitting. Defaults to 100, which will be fine for most plots
- **force** (*boolean*) – If True, the preprocessing and fitting will be executed as a clean run. This will force all intermediate results to be recalculated. Defaults to False

Returns **variogram** – first element is the created lags array second element are the calculated semi-variance values

Return type tuple

describe()
Variogram parameters

Return a dictionary of the variogram parameters.

Returns

Return type dict

distance_difference_plot(*ax=None*, *plot_bins=True*, *show=True*)
Raw distance plot

Plots all absoulte value differences of all point pair combinations over their separating distance, without sorting them into a lag.

Parameters

- **ax** (*None, AxesSubplot*) – If None, a new matplotlib.Figure will be created. In case a Figure was already created, pass the Subplot to use as ax argument.
- **plot_bins** (*bool*) – If True (default) the bin edges will be included into the plot.
- **show** (*bool*) – If True (default), the show method of the Figure will be called before returning the Figure. Can be set to False, to avoid doubled figure rendering in Jupyter notebooks.

Returns

Return type matplotlib.pyplot.Figure

experimental
Experimental Variogram

Array of experimental (empirical) semivariance values. The array length will be aligned to Variogram.bins. The current Variogram.estimator has been used to calculate the values. Depending on the setting of Variogram.harmonize (True | False), either Variogram._experimental or Variogram.isotonic will be returned.

Returns **vario** – Array of the experimental semi-variance values aligned to Variogram.bins.

Return type numpy.ndarray

See also:

`Variogram._experimental`, *`Variogram.isotonic`*

fit (*force=False*, *method=None*, *sigma=None*, ***kwargs*)
Fit the variogram

The fit function will fit the theoretical variogram function to the experimental. The preprocessed distance matrix, pairwise differences and binning will not be recalculated, if already done. This could be forced by setting the force parameter to true.

In case you call fit function directly, with method or sigma, the parameters set on Variogram object instantiation will get overwritten. All other keyword arguments will be passed to scipy.optimize.curve_fit function.

Parameters

- **force** (*bool*) – If set to True, a clean preprocessing of the distance matrix, pairwise differences and the binning will be forced. Default is False.
- **method** (*string*) – A string identifying one of the implemented fitting procedures. Can be one of ['lm', 'trf']:
  - lm: Levenberg-Marquardt algorithms implemented in scipy.optimize.leastsq function.
  - trf: Trust Region Reflective algorithm implemented in scipy.optimize.least_squares(method='trf')
- **sigma** (*string, array*) – Uncertainty array for the bins. Has to have the same dimension as self.bins. Refer to Variogram.fit_sigma for more information.

Returns

Return type void

See also:

`scipy.optimize()`, `scipy.optimize.curve_fit()`, `scipy.optimize.leastsq()`, `scipy.optimize.least_squares()`

fit_sigma
Fitting Uncertainty

Set or calculate an array of observation uncertainties aligned to the Variogram.bins. These will be used to weight the observations in the cost function, which divides the residuals by their uncertainty.

When setting fit_sigma, the array of uncertainties itself can be given, or one of the strings: ['linear', 'exp', 'sqrt', 'sq']. The parameters described below refer to the setter of this property.

Parameters **sigma** (*string, array*) – Sigma can either be an array of discrete uncertainty values, which have to align to the Variogram.bins, or of type string. Then, the weights for fitting are calculated as a function of (lag) distance.

- **sigma='linear'**: The residuals get weighted by the lag distance normalized to the maximum lag distance, denoted as w_n
- **sigma='exp'**: The residuals get weighted by the function: $w = e^{1/w_n}$
- **sigma='sqrt'**: The residuals get weighted by the function: $w = \sqrt{(w_n)}$
- **sigma='sq'**: The residuals get weighted by the function: $w = w_n^2$

Returns

Return type void

Notes

The cost function is defined as:

$$chisq = \sum \frac{r}{\sigma}^2$$

where r are the residuals between the experimental variogram and the modeled values for the same lag. Following this function, small values will increase the influence of that residual, while a very large sigma will cause the observation to be ignored.

See also:

`scipy.optimize.curve_fit`

fitted_model
Fitted Model

Returns a callable that takes a distance value and returns a semivariance. This model is fitted to the current Variogram parameters. The function will be interpreted at return time with the parameters hard-coded into the function code. This makes it way faster than'Variogram.compiled_model'.

Returns **model** – The current semivariance model fitted to the current Variogram model parameters.

Return type callable

isotonic
Return the isotonic harmonized experimental variogram. This means, the experimental variogram is monotonic after harmonization.

The harmonization is done using PAVA algorithm:

Barlow, R., D. Bartholomew, et al. (1972): Statistical Interference Under Order Restrictions. John Wiley and Sons, New York.

Hiterding, A. (2003): Entwicklung hybrider Interpolationsverfahren für den automatisierten Betrieb am Beispiel meteorologischer Größen. Dissertation, Institut für Geoinformatik, Westphälische Wilhelms-Universität Münster, IfGIprints, Münster. ISBN: 3-936616-12-4

TODO: solve the import

Returns np.ndarray, monotonized experimental variogram

lag_classes()
Iterate over the lag classes

Generates an iterator over all lag classes. Can be zipped with Variogram.bins to identify the lag.

Returns

Return type iterable

lag_groups()
Lag class groups

Retuns a mask array with as many elements as self._diff has, identifying the lag class group for each pairwise difference. Can be used to extract all pairwise values within the same lag bin.

Returns

Return type numpy.ndarray

See also:

`Variogram.lag_classes()`

location_trend(*axes=None*)
Location Trend plot

Plots the values over each dimension of the coordinates in a scatter plot. This will visually show correlations between the values and any of the coordinate dimension. If there is a value dependence on the location, this would violate the intrinsic hypothesis. This is a weaker form of stationarity of second order.

Parameters **axes** (*list*) – Can be None (default) or a list of matplotlib.AxesSubplots. If a list is passed, the location trend plots will be plotted on the given instances. Note that then length of the list has to match the dimeonsionality of the coordinates array. In case 3D coordinates are used, three subplots have to be given.

Returns

Return type matplotlib.Figure

mean_residual
Mean Model residuals

Calculates the mean, absoulte deviations between the experimental variogram and theretical model values.

Returns

Return type float

model_deviations()
Model Deviations

Calculate the deviations between the experimental variogram and the recalculated values for the same bins using the fitted theoretical variogram function. Can be utilized to calculate a quality measure for the variogram fit.

Returns **deviations** – first element is the experimental variogram second element are the corresponding values of the theoretical model.

Return type tuple

nrmse
NRMSE

Calculate the normalized root mean squared error between the experimental variogram and the theoretical model values at corresponding lags. Can be used as a fitting quality measure

Returns

Return type float

See also:

Variogram.residuals, *Variogram.rmse*

Notes

The NRMSE is implemented as:

$$NRMSE = \frac{RMSE}{mean(y)}$$

where RMSE is Variogram.rmse and y is Variogram.experimental

nrmse_r
NRMSE

Alternative normalized root mean squared error between the experimental variogram and the theoretical model values at corresponding lags. Can be used as a fitting quality measure.

Returns

Return type float

See also:

Variogram.rmse, *Variogram.nrmse*

Notes

Unlike Variogram.nrmse, nrmse_r is not normalized to the mean of y, but the differece of the maximum y to its mean:

$$NRMSE_r = \frac{RMSE}{max(y) - mean(y)}$$

parameters
Extract just the variogram parameters range, sill and nugget from the self.describe return

Returns

plot (*axes=None*, *grid=True*, *show=True*, *hist=True*)
Variogram Plot

Plot the experimental variogram, the fitted theoretical function and an histogram for the lag classes. The axes attribute can be used to pass a list of AxesSubplots or a single instance to the plot function. Then these Subplots will be used. If only a single instance is passed, the hist attribute will be ignored as only the variogram will be plotted anyway.

Parameters

- **axes** (*list, tuple, array, AxesSubplot or None*) – If None, the plot function will create a new matplotlib figure. Otherwise a single instance or a list of AxesSubplots can be passed to be used. If a single instance is passed, the hist attribute will be ignored.
- **grid** (*bool*) – Defaults to True. If True a custom grid will be drawn through the lag class centers
- **show** (*bool*) – Defaults to True. If True, the show method of the passed or created matplotlib Figure will be called before returning the Figure. This should be set to False, when used in a Notebook, as a returned Figure object will be plotted anyway.
- **hist** (*bool*) – Defaults to True. If False, the creation of a histogram for the lag classes will be suppressed.

Returns

Return type matplotlib.Figure

preprocessing (*force=False*)
Preprocessing function

Prepares all input data for the fit and transform functions. Namely, the distances are calculated and the value differences. Then the binning is set up and bin edges are calculated. If any of the listed subsets are already prepared, their processing is skipped. This behaviour can be changed by the force parameter. This will cause a clean preprocessing.

Parameters **force** (*bool*) – If set to True, all preprocessing data sets will be deleted. Use it in case you need a clean preprocessing.

Returns

Return type void

r

Pearson correlation of the fitted Variogram

Returns

residuals

Model residuals

Calculate the model residuals defined as the differences between the experimental variogram and the theoretical model values at corresponding lag values

Returns

Return type numpy.ndarray

rmse

RMSE

Calculate the Root Mean squared error between the experimental variogram and the theoretical model values at corresponding lags. Can be used as a fitting quality measure.

Returns

Return type float

See also:

Variogram.residuals

Notes

The RMSE is implemented like:

$$RMSE = \sqrt{\frac{\sum_{i=0}^{i=N(x)}(x-y)^2}{N(x)}}$$

set_bin_func (*bin_func*)

Set binning function

Sets a new binning function to be used. The new binning method is set by a string identifying the new function to be used. Can be one of: [‘even’, ‘uniform’].

Parameters **bin_func** (*str*) – Can be one of:

- **’even’**: Use skgstat.binning.even_width_lags for using n_lags lags of equal width up to maxlag.
- **’uniform’**: Use skgstat.binning.uniform_count_lags for using n_lags lags up to maxlag in which the pairwise differences follow a uniform distribution.

Returns

Return type void

See also:

Variogram.bin_func(), skgstat.binning.uniform_count_lags(), skgstat.binning.even_width_lags()

set_dist_function(*func*)
Set distance function

Set the function used for distance calculation. func can either be a callable or a string. The ranked distance function is not implemented yet. strings will be forwarded to the scipy.spatial.distance.pdist function as the metric argument. If func is a callable, it has to return the upper triangle of the distance matrix as a flat array (Like the pdist function).

Parameters **func** (*string, callable*) –

Returns

Return type numpy.array

set_model(*model_name*)
Set model as the new theoretical variogram function.

set_values(*values*)
Set new values

Will set the passed array as new value array. This array has to be of same length as the first axis of the coordinates array. The Variogram class does only accept one dimensional arrays. On success all fitting parameters are deleted and the pairwise differences are recalculated.

Parameters **values** (*numpy.ndarray*) –

Returns

Return type void

See also:

Variogram.values()

to_DataFrame(*n=100*, *force=False*)
Variogram DataFrame

Returns the fitted theoretical variogram as a pandas.DataFrame instance. The n and force parameter control the calaculation, refer to the data funciton for more info.

Parameters

- **n** (*integer*) – length of the lags array to be used for fitting. Defaults to 100, which will be fine for most plots
- **force** (*boolean*) – If True, the preprocessing and fitting will be executed as a clean run. This will force all intermediate results to be recalculated. Defaults to False

Returns

Return type pandas.DataFrame

See also:

Variogram.data()

transform(*x*)
Transform

Transform a given set of lag values to the theoretical variogram function using the actual fitting and preprocessing parameters in this Variogram instance

Parameters **x** (*numpy.array*) – Array of lag values to be used as model input for the fitted theoretical variogram model

Returns

Return type numpy.array

value_matrix

Value matrix

Returns a matrix of pairwise differences in absolute values. The matrix will have the shape (m, m) with m = len(Variogram.values). Note that Variogram.values holds the values themselves, while the value_matrix consists of their pairwise differences.

Returns **values** – Matrix of pairwise absolute differences of the values.

Return type numpy.matrix

See also:

`Variogram._diff`

values

Values property

Array of observations, the variogram is build for. The setter of this property utilizes the Variogram.set_values function for setting new arrays.

Returns **values**

Return type numpy.ndarray

See also:

Variogram.set_values

2.5.2 DirectionalVariogram Class

class skgstat.**DirectionalVariogram**(*coordinates=None*, *values=None*, *estimator='matheron'*, *model='spherical'*, *dist_func='euclidean'*, *bin_func='even'*, *normalize=True*, *fit_method='trf'*, *fit_sigma=None*, *directional_model='triangle'*, *azimuth=0*, *tolerance=45.0*, *bandwidth='q33'*, *use_nugget=False*, *maxlag=None*, *n_lags=10*, *verbose=False*, *harmonize=False*)

DirectionalVariogram Class

Calculates a variogram of the separating distances in the given coordinates and relates them to one of the semivariance measures of the given dependent values.

The direcitonal version of a Variogram will only form paris of points that share a specified spatial relationship.

__init__(*coordinates=None*, *values=None*, *estimator='matheron'*, *model='spherical'*, *dist_func='euclidean'*, *bin_func='even'*, *normalize=True*, *fit_method='trf'*, *fit_sigma=None*, *directional_model='triangle'*, *azimuth=0*, *tolerance=45.0*, *bandwidth='q33'*, *use_nugget=False*, *maxlag=None*, *n_lags=10*, *verbose=False*, *harmonize=False*)

Variogram Class

Directional Variogram. The calculation is not performant and not tested yet.

Parameters

- **coordinates** (*numpy.ndarray*) – Array of shape (m, n). Will be used as m observation points of n-dimensions. This variogram can be calculated on 1 - n dimensional coordinates. In case a 1-dimensional array is passed, a second array of same length containing only zeros will be stacked to the passed one.
- **values** (*numpy.ndarray*) – Array of values observed at the given coordinates. The length of the values array has to match the m dimension of the coordinates array. Will be used to calculate the dependent variable of the variogram.
- **estimator** (*str, callable*) – String identifying the semi-variance estimator to be used. Defaults to the Matheron estimator. Possible values are:
  - matheron [Matheron, default]
  - cressie [Cressie-Hawkins]
  - dowd [Dowd-Estimator]
  - genton [Genton]
  - minmax [MinMax Scaler]
  - entropy [Shannon Entropy]

  If a callable is passed, it has to accept an array of absoulte differences, aligned to the 1D distance matrix (flattened upper triangle) and return a scalar, that converges towards small values for similarity (high covariance).
- **model** (*str*) – String identifying the theoretical variogram function to be used to describe the experimental variogram. Can be one of:
  - spherical [Spherical, default]
  - exponential [Exponential]
  - gaussian [Gaussian]
  - cubic [Cubic]
  - stable [Stable model]
  - matern [Matérn model]
  - nugget [nugget effect variogram]
- **dist_func** (*str*) – String identifying the distance function. Defaults to 'euclidean'. Can be any metric accepted by scipy.spatial.distance.pdist. Additional parameters are not (yet) passed through to pdist. These are accepted by pdist for some of the metrics. In these cases the default values are used.
- **bin_func** (*str*) – String identifying the binning function used to find lag class edges. At the moment there are two possible values: 'even' (default) or 'uniform'. Even will find n_lags bins of same width in the interval [0,maxlag[. 'uniform' will identfy n_lags bins on the same interval, but with varying edges so that all bins count the same amount of observations.
- **normalize** (*bool*) – Defaults to False. If True, the independent and dependent variable will be normalized to the range [0,1].
- **fit_method** (*str*) – String identifying the method to be used for fitting the theoretical variogram function to the experimental. More info is given in the Variogram.fit docs. Can be one of:
  - 'lm': Levenberg-Marquardt algorithm for unconstrained problems. This is the faster algorithm, yet is the fitting of a variogram not unconstrianed.

  - 'trf': Trust Region Reflective function for non-linear constrained problems. The class will set the boundaries itself. This is the default function.

- **fit_sigma** (*numpy.ndarray, str*) – Defaults to None. The sigma is used as measure of uncertainty during variogram fit. If fit_sigma is an array, it has to hold n_lags elements, giving the uncertainty for all lags classes. If fit_sigma is None (default), it will give no weight to any lag. Higher values indicate higher uncertainty and will lower the influcence of the corresponding lag class for the fit. If fit_sigma is a string, a pre-defined function of separating distance will be used to fill the array. Can be one of:
  - 'linear': Linear loss with distance. Small bins will have higher impact.
  - 'exp': The weights decrease by a e-function of distance
  - 'sqrt': The weights decrease by the squareroot of distance
  - 'sq': The weights decrease by the squared distance.

  More info is given in the Variogram.fit_sigma documentation.

- **directional_model** (*string, Polygon*) – The model used for selecting all points fulfilling the directional constraint of the Variogram. A predefined model can be selected by passing the model name as string. Optionally a callable accepting the current local coordinate system and returning a Polygon representing the search area itself can be passed. In this case, the tolerance and bandwidth has to be incorporated by hand into the model. The azimuth is handled by the class. The predefined options are:
  - 'compass': includes points in the direction of the azimuth at given tolerance. The bandwidth parameter will be ignored.
  - 'triangle': constructs a triangle with an angle of tolerance at the point of interest and union an rectangle parallel to azimuth, once the hypotenuse length reaches bandwidth.
  - 'circle': constructs a half circle touching the point of interest, dislocating the center at the distance of bandwidth in the direction of azimuth. The half circle is union with an rectangle parallel to azimuth.

  Visual representations, usage hints and implementation specifics are given in the documentation.

- **azimuth** (*float*) – The azimuth of the directional dependence for this Variogram, given as an angle in **degree**. The East of the coordinate plane is set to be at 0° and is counted clockwise to 180° and counter-clockwise to -180°. Only Points lying in the azimuth of a specific point will be used for forming point pairs.

- **tolerance** (*float*) – The tolerance is given as an angle in **degree**- Points being dislocated from the exact azimuth by half the tolerance will be accepted as well. It's half the tolerance as the point may be dislocated in the positive and negative direction from the azimuth.

- **bandwidth** (*float*) – Maximum tolerance acceptable in **coordinate units**, which is usually meter. Points at higher distances may be far dislocated from the azimuth in terms of coordinate distance, as the tolerance is defined as an angle. THe bandwidth defines a maximum width for the search window. It will be perpendicular to and bisected by the azimuth.

- **use_nugget** (*bool*) – Defaults to False. If True, a nugget effet will be added to all Variogram.models as a third (or fourth) fitting parameter. A nugget is essentially the y-axis interception of the theoretical variogram function.

- **maxlag** (*float, str*) – Can specify the maximum lag distance directly by giving a value larger than 1. The binning function will not find any lag class with an edge larger than

maxlag. If 0 < maxlag < 1, then maxlag is relative and maxlag * max(Variogram.distance) will be used. In case maxlag is a string it has to be one of 'median', 'mean'. Then the median or mean of all Variogram.distance will be used. Note maxlag=0.5 will use half the maximum separating distance, this is not the same as 'median', which is the median of all separating distances

- **n_lags** (*int*) – Specify the number of lag classes to be defined by the binning function.
- **verbose** (*bool*) – Set the Verbosity of the class. Not Implemented yet.
- **harmonize** (*bool*) – this kind of works so far, but will be rewritten (and documented)

_triangle (*local_ref*)
Triangular Search Area

Construct a triangular bounded search area for building directional dependent point pairs. The Search Area will be located onto the current point of interest and the local x-axis is rotated onto the azimuth angle.

Parameters **local_ref** (*numpy.array*) – Array of all coordinates transformed into a local representation with the current point of interest being the origin and the azimuth angle aligned onto the x-axis.

Returns **search_area** – Search Area of triangular shape bounded by the current bandwidth.

Return type Polygon

Notes

The point of interest is C and c is the bandwidth. The angle at C (gamma) is the tolerance. From this, a and then h can be calculated. When rotated into the local coordinate system, the two points needed to build the search area A,B are A := (h, 1/2 c) and B:= (h, -1/2 c)

a can be calculated like:

$$a = \frac{c}{2 * sin\left(\frac{\gamma}{2}\right)}$$

See also:

DirectionalVariogram._compass(), *DirectionalVariogram._circle()*

_circle (*local_ref*)
Circular Search Area

Construct a half-circled bounded search area for building directional dependent point pairs. The Search Area will be located onto the current point of interest and the local x-axis is rotated onto the azimuth angle. The radius of the half-circle is set to half the bandwidth.

Parameters **local_ref** (*numpy.array*) – Array of all coordinates transformed into a local representation with the current point of interest being the origin and the azimuth angle aligned onto the x-axis.

Returns **search_area** – Search Area of half-circular shape bounded by the current bandwidth.

Return type Polygon

Raises ValueError : In case the DirectionalVariogram.bandwidth is None or 0.

See also:

DirectionalVariogram._triangle(), *DirectionalVariogram._compass()*

_compass(*local_ref*)
Compass direction Search Area

Construct a search area for building directional dependent point pairs. The compass search area will **not** be bounded by the bandwidth. It will include all point pairs at the azimuth direction with a given tolerance. The Search Area will be located onto the current point of interest and the local x-axis is rotated onto the azimuth angle.

Parameters **local_ref** (*numpy.array*) – Array of all coordinates transformed into a local representation with the current point of interest being the origin and the azimuth angle aligned onto the x-axis.

Returns **search_area** – Search Area of the given compass direction.

Return type Polygon

Notes

The necessary figure is build by searching for the intersection of a half-tolerance angled line with a vertical line at the maximum x-value. Using polar coordinates, these points (positive and negative half-tolerance angle) are the edges of the search area in the local coordinate system. The radius of a polar coordinate can be calculated as:

$$r = \frac{x}{cos(\alpha/2)}$$

The two bounding points P1 nad P2 (in local coordinates) are then (xmax, y) and (xmax, -y), with xmax being the maximum local x-coordinate representation and y:

$$y = r * sin\left(\frac{\alpha}{2}\right)$$

See also:

DirectionalVariogram._triangle(), *DirectionalVariogram._circle()*

_direction_mask()
Directional Mask

Array aligned to self.distance masking all point pairs which shall be ignored for binning and grouping. The one dimensional array contains all row-wise point pair combinations from the upper or lower triangle of the distance matrix in case either of both is directional.

TODO: This array is not cached. it is used twice, for binning and grouping.

Returns **mask** – Array aligned to self.distance giving for each point pair combination a boolean value whether the point are directional or not.

Return type numpy.array

azimuth
Direction azimuth

Main direction for te selection of points in the formation of point pairs. East of the coordinate plane is defined to be 0° and then the azimuth is set clockwise up to 180°and count-clockwise to -180°.

Parameters **angle** (*float*) – New azimuth angle in **degree**.

Raises ValueError : in case angle < -180° or angle > 180

bandwidth
Tolerance bandwidth

New bandwidth parameter. As the tolerance from azimuth is given as an angle, point pairs at high distances can be far off the azimuth in coordinate distance. The bandwidth limits this distance and has the unnit of the coordinate system.

Parameters **width** (*float*) – Positive coordinate distance.

Raises ValueError : in case width is negative

local_reference_system(*poi*)
Calculate local coordinate system

The coordinates will be transformed into a local reference system that will simplify the directional dependence selection. The point of interest (poi) of the current iteration will be used as origin of the local reference system and the x-axis will be rotated onto the azimuth.

Parameters **poi** (*tuple*) – First two coordinate dimensions of the point of interest. will be used as the new origin

Returns **local_ref** – Array of dimension (m, 2) where m is the length of the coordinates array. Transformed coordinates in the same order as the original coordinates.

Return type numpy.array

search_area(*poi=0*, *ax=None*)
Plot Search Area

Parameters

- **poi** (*integer*) – Point of interest. Index of the coordinate that shall be used to visualize the search area.
- **ax** (*None, matplotlib.AxesSubplot*) – If not None, the Search Area will be plotted into the given Subplot object. If None, a new matplotlib Figure will be created and returned

Returns

Return type plot

set_directional_model(*model_name*)
Set new directional model

The model used for selecting all points fulfilling the directional constraint of the Variogram. A predefined model can be selected by passing the model name as string. Optionally a function can be passed that accepts the current local coordinate system and returns a Polygon representing the search area. In this case, the tolerance and bandwidth has to be incorporated by hand into the model. The azimuth is handled by the class. The predefined options are:

- **'compass': includes points in the direction of the azimuth at given** tolerance. The bandwidth parameter will be ignored.
- 'triangle': constructs a triangle with an angle of tolerance at the point of interest and union an rectangle parallel to azimuth, once the hypotenuse length reaches bandwidth.
- 'circle': constructs a half circle touching the point of interest, dislocating the center at the distance of bandwidth in the direction of azimuth. The half circle is union with an rectangle parallel to azimuth.

Visual representations, usage hints and implementation specifics are given in the documentation.

Parameters **model_name** (*string, callable*) – The name of the predefined model (string) or a function that accepts the current local coordinate system and returns a Polygon of the search area.

tolerance

Azimuth tolerance

Tolerance angle of how far a point can be off the azimuth for being still counted as directional. A tolerance angle will be applied to the azimuth angle symmetrically.

Parameters **angle** (*float*) – New tolerance angle in **degree**. Has to meet 0 <= angle <= 360.

Raises ValueError : in case angle < 0 or angle > 360

2.5.3 SpaceTimeVariogram class

class skgstat.**SpaceTimeVariogram**(*coordinates*, *values*, *xdist_func='euclidean'*, *tdist_func='euclidean'*, *x_lags=10*, *t_lags='max'*, *maxlag=None*, *xbins='even'*, *tbins='even'*, *estimator='matheron'*, *use_nugget=False*, *verbose=False*)

__init__(*coordinates*, *values*, *xdist_func='euclidean'*, *tdist_func='euclidean'*, *x_lags=10*, *t_lags='max'*, *maxlag=None*, *xbins='even'*, *tbins='even'*, *estimator='matheron'*, *use_nugget=False*, *verbose=False*)

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

build_marginal_variograms()

build marginal Variogram classes

The two marginal variograms for space and time axis will be initialized and added to this instance. Both are an instance of skgstat.Variogram in order to model them properly. Use these classes to well working valid models to the marginal Variograms before modeling the space-time model. The two objects will be available as SpaceTimeVariogram.XMarginal and SpaceTimeVariogram.TMarginal.

contour(*ax=None*, *zoom_factor=100.0*, *levels=10*, *colors='k'*, *linewidths=0.3*, *method='fast'*, ***kwargs*)

Variogram 2D contour plot

Plot a 2D contour plot of the experimental variogram. The experimental semi-variance values are spanned over a space - time lag meshgrid. This grid is (linear) interpolated onto the given resolution for visual reasons. Then, contour lines are caluclated from the denser grid. Their number can be specified by *levels*.

Parameters

- **ax** (*matplotlib.AxesSubplot, None*) – If None a new matplotlib.Figure will be created, otherwise the plot will be rendered into the given subplot.
- **zoom_factor** (*float*) – The experimental variogram will be interpolated onto a regular grid for visual reasons. The density of this plot can be set by zoom_factor. A factor of 10 will enlarge each of the axes by 10. Higher zoom_factors result in smoother contours, but are expansive in calculation time.
- **levels** (*int*) – Number of levels to be formed for finding contour lines. More levels result in more detailed plots, but are expansive in terms of calculation time.
- **colors** (*str, list*) – Will be passed down to matplotlib.pyplot.contour as *c* parameter.
- **linewidths** (*float, list*) – Will be passed down to matplotlib.pyplot.contour as *linewidths* parameter.

- **method** (*str*) – The method used for densifying the meshgrid. Can be one of 'fast' or 'precise'. Fast will use the scipy.ndimage.zoom method to incresae the node density. This is fast, but cannot interpolate *behind* any NaN occurance. 'Precise' performs an actual linear interpolation between the nodes using scipy.interpolate.griddata. This takes more time, but the result is less smoothed out.
- **kwargs** (*dict*) – Other arguments that can be specific to *contour* or *contourf* type. Accepts *xlabel*, *ylabel*, *xlim* and *ylim* as of this writing.

Returns **fig** – The Figure object used for rendering the contour plot.

Return type matplotlib.Figure

See also:

SpaceTimeVariogram.contourf()

contourf(*ax=None*, *zoom_factor=100.0*, *levels=10*, *cmap='RdYlBu_r'*, *method='fast'*, ***kwargs*)

Variogram 2D filled contour plot

Plot a 2D filled contour plot of the experimental variogram. The experimental semi-variance values are spanned over a space - time lag meshgrid. This grid is (linear) interpolated onto the given resolution for visual reasons. Then, contour lines are caluclated from the denser grid. Their number can be specified by *levels*. Finally, each contour region is filled with a color supplied by the specified *cmap*.

Parameters

- **ax** (*matplotlib.AxesSubplot, None*) – If None a new matplotlib.Figure will be created, otherwise the plot will be rendered into the given subplot.
- **zoom_factor** (*float*) – The experimental variogram will be interpolated onto a regular grid for visual reasons. The density of this plot can be set by zoom_factor. A factor of 10 will enlarge each of the axes by 10. Higher zoom_factors result in smoother contours, but are expansive in calculation time.
- **levels** (*int*) – Number of levels to be formed for finding contour lines. More levels result in more detailed plots, but are expansive in terms of calculation time.
- **cmap** (*str*) – Will be passed down to matplotlib.pyplot.contourf as *cmap* parameter. Can be any valid color range supported by matplotlib.
- **method** (*str*) – The method used for densifying the meshgrid. Can be one of 'fast' or 'precise'. Fast will use the scipy.ndimage.zoom method to incresae the node density. This is fast, but cannot interpolate *behind* any NaN occurance. 'Precise' performs an actual linear interpolation between the nodes using scipy.interpolate.griddata. This takes more time, but the result is less smoothed out.
- **kwargs** (*dict*) – Other arguments that can be specific to *contour* or *contourf* type. Accepts *xlabel*, *ylabel*, *xlim* and *ylim* as of this writing.

Returns **fig** – The Figure object used for rendering the contour plot.

Return type matplotlib.Figure

See also:

SpaceTimeVariogram.contour()

create_TMarginal()

Create an instance of skgstat.Variogram for the time marginal variogram by arranging the coordinates and values and infer parameters from this SpaceTimeVariogram instance.

create_XMarginal()
Create an instance of skgstat.Variogram for the space marginal variogram by arranging the coordinates and values and infer parameters from this SpaceTimeVariogram instance.

distance
Distance matrices

Returns both the space and time distance matrix. This property is equivalent to two separate calls of *xdistance* and *tdistance*.

Returns distance matrices – Returns a tuple of the two distance matrices in space and time. Each distance matrix is a flattened upper triangle of the distance matrix squareform in row orientation.

Return type (numpy.array, numpy.array)

experimental
Experimental Variogram

Returns an experimental variogram for the given data. The semivariances are arranged over the spatial binning as defined in SpaceTimeVariogram.xbins and temporal binning defined in SpaceTimeVariogram.tbins.

Returns variogram – Returns an two dimensional array of semivariances over space on the first axis and time over the second axis.

Return type numpy.ndarray

get_marginal(*axis*, *lag=0*)
Marginal Variogram

Returns the marginal experimental variogram of axis for the given lag on the other axis. Axis can either be 'space' or 'time'. The parameter lag specifies the index of the desired lag class on the other axis.

Parameters

- **axis** (*str*) – The axis a marginal variogram shall be calculated for. Can either be 'space' or 'time'.
- **lag** (*int*) – Index of the lag class group on the other axis to be used. In case this is 0, this is often considered to be *the* marginal variogram of the axis.

Returns variogram – Marginal variogram of the given axis

Return type numpy.array

lag_classes()
Iterator over all lag classes

Returns an iterator over all lag classes by aligning all time lags over all space lags. This means that it will yield all time lag groups for a space lag of index 0 at first and then iterate the space lags.

Returns

Return type iterator

lag_groups(*axis*)
Lag class group mask array

Returns a mask array for the given axis (either 'space' or 'time'). It will have as amany elements as the respective distance matrices. **Unlike the base Variogram class, it does not mask the array of pairwise differences.**. It will mask the distance matrix of the respective axis.

Parameters axis (*str*) – Can either be 'space' or 'time'. Specifies the axis the mask array shall be returned for.

Returns **masK_array** – mask array that identifies the lag class group index for each pair of points on the given axis.

Return type numpy.array

marginals(*plot=True*, *axes=None*, *sharey=True*, ***kwargs*)
Plot marginal variograms

Plots the two marginal variograms into a new or existing figure. The space marginal variogram is defined to be the variogram of temporal lag class 0, while the time marginal variogram uses only spatial lag class 0. In case the expected variability is not of same magnitude, the sharey parameter should be set to `False` in order to use separated y-axes.

Parameters

- **plot** (*bool*) – If set to False, no matplotlib.Figure will be returned. Instead a tuple of the two marginal experimental variogram values is returned.
- **axes** (*list*) – Is either `None` to create a new matplotlib.Figure. Otherwise it has to be a list of two matplotlib.AxesSubplot instances, which will then be used for plotting.
- **sharey** (*bool*) – If True (default), the two marginal variograms will share their y-axis to increase comparability. Should be set to False in the variances are of different magnitude.
- **kwargs** (*dict*) – Only kwargs accepted is `figsize`, if ax is None. Anything else will be ignored.

Returns

- **variograms** (*tuple*) – If plot is False, a tuple of numpy.arrays are returned. These are the two experimental marginal variograms.
- **plots** (*matplotlib.Figure*) – If plot is True, the matplotlib.Figure will be returned.

plot(*kind='scatter'*, *ax=None*, ***kwargs*)
Plot the experimental variogram

At the current version the SpaceTimeVariogram class is not capable of modeling a spe-time variogram function, therefore all plots will only show the experimental variogram. As the experimental space-time semivariance is depending on a space and a time lag, one would basically need a 3D scatter plot, which is the default plot. However, 3D plots can be, especially for scientific usage, a bit problematic. Therefore the plot function can plot a variety of 3D and 2D plots.

Parameters

- **kind** (*str*) – Has to be one of:
  - **scatter**
  - **surface**
  - **contour**
  - **contourf**
  - **matrix**
  - **marginals**
- **ax** (*matplotlib.AxesSubplot, mpl_toolkits.mplot3d.Axes3D, None*) – If None, the function will create a new figure and suitable Axes. Else, the Axes object can be passed to plot the variogram into an existing figure. In this case, one has to pass the correct type of Axes, whether it's a 3D or 2D kind of a plot.

- **kwargs** (*dict*) – All keyword arguments are passed down to the actual plotting function. Refer to their documentation for a more detailed description.

Returns fig

Return type matplotlib.Figure

See also:

SpaceTimeVariogram.scatter(), *SpaceTimeVariogram.surface()*, *SpaceTimeVariogram.marginals()*

preprocessing(*force=False*)
Preprocessing

Start all necessary calculation jobs needed to derive an experimental variogram. This hasto be present before the model fitting can be done. The force parameter will make all calculation functions to delete all cached intermediate results and make a clean calculation.

Parameters **force** (*bool*) – If True, all cached intermediate results will be deleted and a clean calculation will be done.

scatter(*ax=None*, *elev=30*, *azim=220*, *c='g'*, *depthshade=True*, ***kwargs*)
3D Scatter Variogram

Plot the experimental variogram into a 3D matplotlib.Figure. The two variogram axis (space, time) will span a meshgrid over the x and y axis and the semivariance will be plotted as z value over the respective space and time lag coordinate.

Parameters

- **ax** (*mpl_toolkits.mplot3d.Axes3D, None*) – If ax is None (default), a new Figure and Axes instance will be created. If ax is given, this instance will be used for the plot.
- **elev** (*int*) – The elevation of the 3D plot, which is a rotation over the xy-plane.
- **azim** (*int*) – The azimuth of the 3D plot, which is a rotation over the z-axis.
- **c** (*str*) – Color of the scatter points, will be passed to the matplotlib `c` argument. The function also accepts `color` as an alias.
- **depthshade** (*bool*) – If True, the scatter points will change their color according to the distance from the viewport for illustration reasons.
- **kwargs** (*dict*) – Other kwargs accepted are only `color` as an alias for `c` and `figsize`, if ax is None. Anything else will be ignored.

Returns fig

Return type matplotlib.Figure

Examples

In case an ax shall be passed to the function, note that this plot requires an AxesSubplot, that is capable of creating a 3D plot. This can be done like:

```
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
```

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```
# STV is an instance of SpaceTimeVariogram
STV.scatter(ax=ax)
```

See also:

SpaceTimeVariogram.surface()

set_bin_func(*bin_func*, *axis*)
Set binning function

Set a new binning function to either the space or time axis. Both axes support the methods: ['even', 'uniform']:

- **'even'**, create even width bins
- **'uniform'**, create bins of uniform distribution

Parameters

- **bin_func** (*str*) – Sepcifies the function to be loaded. Can be either 'even' or 'uniform'.
- **axis** (*str*) – Specifies the axis to be used for binning. Can be either 'space' or 'time', or one of the two shortcuts 's' and 't'

See also:

skgstat.binning.even_width_lags(), skgstat.binning.uniform_count_lags()

set_tdist_func(*func_name*)
Set new space distance function

Set a new function for calculating the distance matrix in the space dimension. At the moment only strings are supported. Will be passed to scipy.spatical.distance.pdist as 'metric' attribute.

Parameters **func_name** (*str*) – The name of the function used to calculate the pairwise distances. Will be passed to scipy.spatial.distance.pdist as the 'metric' attribute.

Raises ValueError : in case a non-string argument is passed.

set_values(*values*)
Set new values

The values should be an (m, n) array with m matching the size of coordinates first dimension and n is the time dimension.

Raises

- *ValueError : in case n <= 1 or values are not an array of correct* – dimensionality
- AttributeError : in case values cannot be converted to a numpy.array

set_xdist_func(*func_name*)
Set new space distance function

Set a new function for calculating the distance matrix in the space dimension. At the moment only strings are supported. Will be passed to scipy.spatical.distance.pdist as 'metric' attribute.

Parameters **func_name** (*str*) – The name of the function used to calculate the pairwise distances. Will be passed to scipy.spatial.distance.pdist as the 'metric' attribute.

Raises ValueError : in case a non-string argument is passed.

surface (*ax=None*, *elev=30*, *azim=220*, *color='g'*, *alpha=0.5*, ***kwargs*)
3D Scatter Variogram

Plot the experimental variogram into a 3D matplotlib.Figure. The two variogram axis (space, time) will span a meshgrid over the x and y axis and the semivariance will be plotted as z value over the respective space and time lag coordinate. Unlike *scatter* the semivariance will not be scattered as points but rather as a surface plot. The surface is approximated by (Delauney) triangulation of the z-axis.

Parameters

- **ax** (*mpl_toolkits.mplot3d.Axes3D, None*) – If ax is None (default), a new Figure and Axes instance will be created. If ax is given, this instance will be used for the plot.
- **elev** (*int*) – The elevation of the 3D plot, which is a rotation over the xy-plane.
- **azim** (*int*) – The azimuth of the 3D plot, which is a rotation over the z-axis.
- **color** (*str*) – Color of the scatter points, will be passed to the matplotlib `color` argument. The function also accepts `c` as an alias.
- **alpha** (*float*) – Sets the transparency of the surface as 0 <= alpha <= 1, with 0 being completely transparent.
- **kwargs** (*dict*) – Other kwargs accepted are only `color` as an alias for `c` and `figsize`, if ax is None. Anything else will be ignored.

Returns **fig**

Return type matplotlib.Figure

Notes

In case an ax shall be passed to the function, note that this plot requires an AxesSubplot, that is capable of creating a 3D plot. This can be done like:

```
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

# STV is an instance of SpaceTimeVariogram
STV.surface(ax=ax)
```

See also:

SpaceTimeVariogram.scatter()

tbins
Temporal binning

Returns the bin edges over the temporal axis. These can be used to align the temporal lag class grouping to actual time lags. The length of the array matches the number of temporal lag classes.

Returns **bins** – Returns the edges of the current temporal binning.

Return type numpy.array

tdistance
Time distance

Returns a distance matrix containing the distance of all observation points in time. The time 'coordiantes' are created from the values multidimensional array, where the second dimension is assumed to be time. The unit will be time steps.

Returns **tdistance** – 1D-array of the upper triangle of a squareform representation of the distance matrix.

Return type numpy.array

values
Values

The SpaceTimeVariogram stores (and needs) the observations as a two dimensional array. The first axis (rows) need to match the coordinate array, but instead of containing one value for each location, the values shall contain a time series per location.

Returns **values** – Returns a two dimensional array of all observations. The first dimension (rows) matches the coordinate array and the second axis contains the time series for each observation point.

Return type numpy.array

xbins
Spatial binning

Returns the bin edges over the spatial axis. These can be used to align the spatial lag class grouping to actual distance lags. The length of the array matches the number of spatial lag classes.

Returns **bins** – Returns the edges of the current spatial binning.

Return type numpy.array

xdistance
Distance matrix (space)

Return the upper triangle of the squareform pairwise distance matrix.

Returns **xdistance** – 1D-array of the upper triangle of a squareform representation of the distance matrix.

Return type numpy.array

2.5.4 Estimator Functions

Scikit-GStat implements various semi-variance estimators. These fucntions can be found in the skgstat.estimators submodule. Each of these functions can be used independently from Variogram class. In this case the estimator is expecting an array of pairwise differences to calculate the semi-variance. Not the values themselves.

Matheron

skgstat.estimators.**matheron**()
Matheron Semi-Variance

Calculates the Matheron Semi-Variance from an array of pairwise differences. Returns the semi-variance for the whole array. In case a semi-variance is needed for multiple groups, this function has to be mapped on each group. That is the typical use case in geostatistics.

Parameters **x** (*numpy.ndarray*) – Array of pairwise differences. These values should be the distances between pairwise observations in value space. If xi and x[i+h] fall into the h separating distance class, x should contain abs(xi - x[i+h]) as an element.

Returns

Return type numpy.float64

Notes

This implementation follows the original publication[1] and the notes on their application[2]. Following the 1962 publication[1], the semi-variance is calculated as:

$$\gamma(h) = \frac{1}{2N(h)} * \sum_{i=1}^{N(h)} (x)^2$$

with:

$$x = Z(x_i) - Z(x_{i+h})$$

where x is exactly the input array x.

References

Cressie

skgstat.estimators.**cressie**()

Cressie-Hawkins Semi-Variance

Calculates the Cressie-Hawkins Semi-Variance from an array of pairwise differences. Returns the semi-variance for the whole array. In case a semi-variance is needed for multiple groups, this function has to be mapped on each group. That is the typical use case in geostatistics.

Parameters **x** (*numpy.ndarray*) – Array of pairwise differences. These values should be the distances between pairwise observations in value space. If xi and x[i+h] fall into the h separating distance class, x should contain abs(xi - x[i+h]) as an element.

Returns

Return type numpy.float64

Notes

This implementation is done after the publication by Cressie and Hawkins from 1980[3]:

$$2\gamma(h) = \frac{(\frac{1}{N(h)} \sum_{i=1}^{N(h)} |x|^{0.5})^4}{0.457 + \frac{0.494}{N(h)} + \frac{0.045}{N^2(h)}}$$

with:

$$x = Z(x_i) - Z(x_{i+h})$$

where x is exactly the input array x.

[1] Matheron, G. (1962): Traité de Géostatistique Appliqué, Tonne 1. Memoires de Bureau de Recherches Géologiques et Miniéres, Paris.
[2] Matheron, G. (1965): Les variables regionalisées et leur estimation. Editions Masson et Cie, 212 S., Paris.
[3] Cressie, N., and D. Hawkins (1980): Robust estimation of the variogram. Math. Geol., 12, 115-125.

References

Dowd

skgstat.estimators.**dowd**(*x*)
Dowd semi-variance

Calculates the Dowd semi-variance from an array of pairwise differences. Returns the semi-variance for the whole array. In case a semi-variance is needed for multiple groups, this function has to be mapped on each group. That is the typical use case in geostatistics.

Parameters **x** (*numpy.ndarray*) – Array of pairwise differences. These values should be the distances between pairwise observations in value space. If xi and x[i+h] fall into the h separating distance class, x should contain abs(xi - x[i+h]) as an element.

Returns

Return type numpy.float64

Notes

The Dowd estimator is based on the median of all pairwise differences in each lag class and is therefore robust to exteme values at the cost of variability. This implementation follows Dowd's publication[4]:

$$2\gamma(h) = 2.198 * median(x)^2$$

with:

$$x = Z(x_i) - Z(x_{i+h})$$

where x is exactly the input array x.

References

Genton

skgstat.estimators.**genton**()
Genton robust semi-variance estimator

Return the Genton semi-variance of the given sample x. Genton is a highly robust varigram estimator, that is designed to be location free and robust on extreme values in x. Genton is based on calculating kth order statistics and will for large data sets be close or equal to the 25% quartile of all ordered point pairs in X.

Parameters **x** (*numpy.ndarray*) – Array of pairwise differences. These values should be the distances between pairwise observations in value space. If xi and x[i+h] fall into the h separating distance class, x should contain abs(xi - x[i+h]) as an element.

Returns

Return type numpy.float64

[4] Dowd, P. A., (1984): The variogram and kriging: Robust and resistant estimators, in Geostatistics for Natural Resources Characterization. Edited by G. Verly et al., pp. 91 - 106, D. Reidel, Dordrecht.

Notes

The Genton estimator is described in great detail in the original publication[5] and is defined as:

$$Q_{N_h} = 2.2191\{|V_i(h) - V_j(h)|; i < j\}_{(k)}$$

and

$$k = \binom{[N_h/2] + 1}{2}$$

and

$$q = \binom{N_h}{2}$$

where k is the kth quantile of all q point pairs. For large N (k/q) will be close to 0.25. For N >= 500, (k/q) is close to 0.25 by two decimals and will therefore be set to 0.5 and the two binomial coefficients k, q are not calculated.

References

Shannon Entropy

skgstat.estimators.**entropy**(*x*, *bins=None*)

Shannon Entropy estimator

Calculates the Shannon Entropy H as a variogram estimator. It is highly recommended to calculate the bins and explicitly set them as a list. In case this function is called for more than one lag class in a variogram, setting bins to None would result in different bin edges in each lag class. This would be very difficult to interpret.

Parameters

- **x** (*numpy.ndarray*) – Array of pairwise differences. These values should be the distances between pairwise observations in value space. If xi and x[i+h] fall into the h separating distance class, x should contain abs(xi - x[i+h]) as an element.
- **bins** (*int, list, str*) – list of the bin edges used to calculate the empirical distribution of x. If bins is a list, these values are used directly. In case bins is a integer, as many even width bins will be calculated between the minimum and maximum value of x. In case bins is a string, it will be passed as bins argument to numpy.histograms function.

Returns **entropy** – Shannon entropy of the given pairwise differences.

Return type numpy.float64

Notes

MinMax

Warning: This is an experimental semi-variance estimator. It is heavily influenced by extreme values and outliers. That behaviour is usually not desired in geostatistics.

[5] Genton, M. G., (1998): Highly robust variogram estimation, Math. Geol., 30, 213 - 221.

skgstat.estimators.**minmax**(*x*)
Minimum - Maximum Estimator

Returns a custom value. This estimator is the difference of maximum and minimum pairwise differences, normalized by the mean. MinMax will be very sensitive to extreme values.

Do only use this estimator, in case you know what you are doing. It is experimental and might change its behaviour in a future version.

Parameters **x** (*numpy.ndarray*) – Array of pairwise differences. These values should be the distances between pairwise observations in value space. If xi and x[i+h] fall into the h separating distance class, x should contain abs(xi - x[i+h]) as an element.

Returns

Return type numpy.float64

Percentile

Warning: This is an experimental semi-variance estimator. It uses just a percentile of the given pairwise differences and does not bear any information about their variance.

skgstat.estimators.**percentile**(*x*, *p=50*)
Percentile estimator

Returns a given percentile as semi-variance. Do only use this estimator, in case you know what you are doing.

Do only use this estimator, in case you know what you are doing. It is experimental and might change its behaviour in a future version.

Parameters

- **x** (*numpy.ndarray*) – Array of pairwise differences. These values should be the distances between pairwise observations in value space. If xi and x[i+h] fall into the h separating distance class, x should contain abs(xi - x[i+h]) as an element.
- **p** (*int*) – Desired percentile. Should be given as whole numbers 0 < p < 100.

Returns

Return type np.float64

2.5.5 Variogram models

Scikit-GStat implements different theoretical variogram functions. These model functions expect a single lag value or an array of lag values as input data. Each function has at least a parameter *a* for the effective range and a parameter *c0* for the sill. The nugget parameter *b* is optinal and will be set to $b := 0$ if not given.

Spherical model

skgstat.models.**spherical**(*h*, *r*, *c0*, *b=0*)
Spherical Variogram function

Implementation of the spherical variogram function. Calculates the dependent variable for a given lag (h). The nugget (b) defaults to be 0.

Parameters

- **h** (*float*) – Specifies the lag of separating distances that the dependent variable shall be calculated for. It has to be a positive real number.
- **r** (*float*) – The effective range. Note this is not the range parameter! However, for the spherical variogram the range and effective range are the same.
- **c0** (*float*) – The sill of the variogram, where it will flatten out. The function will not return a value higher than C0 + b.
- **b** (*float*) – The nugget of the variogram. This is the value of independent variable at the distance of zero. This is usually attributed to non-spatial variance.

Returns **gamma** – Unlike in most variogram function formulas, which define the function for $2 * \gamma$, this function will return γ only.

Return type numpy.float64

Notes

The implementation follows[6]:

$$\gamma = b + C_0 * \left(1.5 * \frac{h}{r} - 0.5 * \frac{h}{r}^3\right)$$

if $h < r$, and

$$\gamma = b + C_0$$

else. r is the effective range, which is in case of the spherical variogram just a.

References

Exponential model

skgstat.models.**exponential**(*h*, *r*, *c0*, *b=0*)

Exponential Variogram function

Implementation of the exponential variogram function. Calculates the dependent variable for a given lag (h). The nugget (b) defaults to be 0.

Parameters

- **h** (*float*) – Specifies the lag of separating distances that the dependent variable shall be calculated for. It has to be a positive real number.
- **r** (*float*) – The effective range. Note this is not the range parameter! For the exponential variogram function the range parameter a is defined to be $a = \frac{r}{3}$. The effective range is the lag where 95% of the sill are exceeded. This is needed as the sill is only approached asymptotically by an exponential function.
- **c0** (*float*) – The sill of the variogram, where it will flatten out. The function will not return a value higher than C0 + b.
- **b** (*float*) – The nugget of the variogram. This is the value of independent variable at the distance of zero. This is usually attributed to non-spatial variance.

[6] Burgess, T. M., & Webster, R. (1980). Optimal interpolation and isarithmic mapping of soil properties. I.The semi-variogram and punctual kriging. Journal of Soil and Science, 31(2), 315–331, http://doi.org/10.1111/j.1365-2389.1980.tb02084.x

Returns **gamma** – Unlike in most variogram function formulas, which define the function for $2 * \gamma$, this function will return γ only.

Return type numpy.float64

Notes

The implementation following[7] and[8] is as:

$$\gamma = b + C_0 * \left(1 - e^{-\frac{h}{a}}\right)$$

a is the range parameter, that can be calculated from the effective range r as: $a = \frac{r}{3}$.

References

Gaussian model

skgstat.models.**gaussian**(*h*, *r*, *c0*, *b=0*)

Gaussian Variogram function

Implementation of the Gaussian variogram function. Calculates the dependent variable for a given lag (h). The nugget (b) defaults to be 0.

Parameters

- **h** (*float*) – Specifies the lag of separating distances that the dependent variable shall be calculated for. It has to be a positive real number.
- **r** (*float*) – The effective range. Note this is not the range parameter! For the exponential variogram function the range parameter a is defined to be $a = \frac{r}{3}$. The effetive range is the lag where 95% of the sill are exceeded. This is needed as the sill is only approached asymptotically by an exponential function.
- **c0** (*float*) – The sill of the variogram, where it will flatten out. The function will not return a value higher than C0 + b.
- **b** (*float*) – The nugget of the variogram. This is the value of independent variable at the distance of zero. This is usually attributed to non-spatial variance.

Returns **gamma** – Unlike in most variogram function formulas, which define the function for $2 * \gamma$, this function will return γ only.

Return type numpy.float64

Notes

This implementation follows[9]:

$$\gamma = b + c_0 * \left(1 - e^{-\frac{h^2}{a^2}}\right)$$

a is the range parameter, that can be calculated from the effective range r as:

$$a = \frac{r}{2}$$

[7] Cressie, N. (1993): Statistics for spatial data. Wiley Interscience.
[8] Chiles, J.P., Delfiner, P. (1999). Geostatistics. Modeling Spatial Uncertainty. Wiley Interscience.
[9] Chiles, J.P., Delfiner, P. (1999). Geostatistics. Modeling Spatial Uncertainty. Wiley Interscience.

References

Cubic model

skgstat.models.**cubic**(*h*, *r*, *c0*, *b=0*)

Cubic Variogram function

Implementation of the Cubic variogram function. Calculates the dependent variable for a given lag (h). The nugget (b) defaults to be 0.

Parameters

- **h** (*float*) – Specifies the lag of separating distances that the dependent variable shall be calculated for. It has to be a positive real number.
- **r** (*float*) – The effective range. Note this is not the range parameter! However, for the cubic variogram the range and effective range are the same.
- **c0** (*float*) – The sill of the variogram, where it will flatten out. The function will not return a value higher than C0 + b.
- **b** (*float*) – The nugget of the variogram. This is the value of independent variable at the distance of zero. This is usually attributed to non-spatial variance.

Returns **gamma** – Unlike in most variogram function formulas, which define the function for $2 * \gamma$, this function will return γ only.

Return type numpy.float64

Notes

This implementation is like:

$$\gamma = b + c_0 * \left[7 * \left(\frac{h^2}{a^2}\right) - \frac{35}{4} * \left(\frac{h^3}{a^3}\right) + \frac{7}{2} * \left(\frac{h^5}{a^5}\right) - \frac{3}{4} * \left(\frac{h^7}{a^7}\right)\right]$$

a is the range parameter. For the cubic function, the effective range and range parameter are the same.

Stable model

skgstat.models.**stable**(*h*, *r*, *c0*, *s*, *b=0*)

Stable Variogram function

Implementation of the stable variogram function. Calculates the dependent variable for a given lag (h). The nugget (b) defaults to be 0.

Parameters

- **h** (*float*) – Specifies the lag of separating distances that the dependent variable shall be calculated for. It has to be a positive real number.
- **r** (*float*) – The effective range. Note this is not the range parameter! For the stable variogram function the range parameter a is defined to be $a = \frac{r}{\sqrt[s]{3}}$. The effective range is the lag where 95% of the sill are exceeded. This is needed as the sill is only approached asymptotically by the e-function part of the stable model.
- **c0** (*float*) – The sill of the variogram, where it will flatten out. The function will not return a value higher than C0 + b.

- **s** (*float*) – Shape parameter. For s <= 2 the model will be shaped more like a exponential or spherical model, for s > 2 it will be shaped most like a Gaussian function.
- **b** (*float*) – The nugget of the variogram. This is the value of independent variable at the distance of zero. This is usually attributed to non-spatial variance.

Returns **gamma** – Unlike in most variogram function formulas, which define the function for $2 * \gamma$, this function will return γ only.

Return type numpy.float64

Notes

The implementation is:

$$\gamma = b + C_0 * \left(1. - e^{-\frac{h}{a}^s}\right)$$

a is the range parameter and is calculated from the effective range r as:

$$a = \frac{r}{3^{\frac{1}{s}}}$$

Matérn model

skgstat.models.**matern**(*h*, *r*, *c0*, *s*, *b=0*)

Matérn Variogram function

Implementation of the Matérn variogram function. Calculates the dependent variable for a given lag (h). The nugget (b) defaults to be 0.

Parameters

- **h** (*float*) – Specifies the lag of separating distances that the dependent variable shall be calculated for. It has to be a positive real number.
- **r** (*float*) – The effective range. Note this is not the range parameter! For the Matérn variogram function the range parameter a is defined to be $a = \frac{r}{2}$. The effective range is the lag where 95% of the sill are exceeded. This is needed as the sill is only approached asymptotically by Matérn model.
- **c0** (*float*) – The sill of the variogram, where it will flatten out. The function will not return a value higher than C0 + b.
- **s** (*float*) – Smoothness parameter. The smoothness parameter can shape a smooth or rough variogram function. A value of 0.5 will yield the exponential function, while a smoothness of +inf is exactly the Gaussian model. Typically a value of 10 is close enough to Gaussian shape to simulate its behaviour. Low values are considered to be 'smooth', while larger values are considered to describe a 'rough' random field.
- **b** (*float*) – The nugget of the variogram. This is the value of independent variable at the distance of zero. This is usually attributed to non-spatial variance.

Returns **gamma** – Unlike in most variogram function formulas, which define the function for $2 * \gamma$, this function will return γ only.

Return type numpy.float64

Notes

The formula and references will follow.

2.5.6 Kriging Class

class skgstat.**OrdinaryKriging**(*variogram*, *min_points=5*, *max_points=15*, *mode='exact'*, *precision=100*, *solver='inv'*, *n_jobs=1*, *perf=False*)

__init__(*variogram*, *min_points=5*, *max_points=15*, *mode='exact'*, *precision=100*, *solver='inv'*, *n_jobs=1*, *perf=False*)

Ordinary Kriging routine

Ordinary kriging estimator derived from the given *Variogram <skgstat.Variogram>* class. To calculate estimations for unobserved locations, an instance of this class can either be called, or the *OrdinaryKriging.transform* method can be used.

Parameters

- **variogram** (Variogram) – Variogram used to build the kriging matrix. Make sure that this instance is describing the spatial dependence in the data well, otherwise the kriging estimation will most likely produce bad estimations.
- **min_points** (*int*) – Minimum amount of points, that have to lie within the variogram's range. In case not enough points are available, the estimation will be rejected and a null value will be estimated.
- **max_points** (*int*) – Maximum amount of points, that will be considered for the estimation of one unobserved location. In case more points are available within the variogram's range, only the *max_points* closest will be used for estimation. Note that the kriging matrix will be an max_points x max_points matrix and large numbers do significantly increase the calculation time.
- **mode** (*str*) – Has to be one of 'exact' or 'estimate'. In exact mode (default) the variogram matrix will be calculated from scratch in each iteration. This gives an exact solution, but it is also slower. In estimate mode, a set of semivariances is pre-calculated and the closest value will be used. This is significantly faster, but the estimation quality is dependent on the given precision.
- **precision** (*int*) – Only needed if *mode='estimate'*. This is the number of pre-calculated in-range semivariances. If chosen too low, the estimation will be off, if too high the performance gain is limited.
- **solver** (*str*) – Do not change this argument
- **n_jobs** (*int*) – Number of processes to be started in multiprocessing.
- **perf** (*bool*) – If True, the different parts of the algorithm will record their processing time. This is meant to be used for optimization and will be removed in a future version. Do not rely on this argument.

transform(**x*)

Kriging

returns an estimation of the observable for the given unobserved locations. Each coordinate dimension should be a 1D array.

Parameters **x** (*numpy.array*) – One 1D array for each coordinate dimension. Typically two or three array, x, y, (z) are passed for 2D and 3D Kriging

Returns **Z** – Array of estimates

Return type numpy.array

2.6 Changelog

2.6.1 Version 0.2.6

- [OrdinaryKriging]: widely enhanced the class in terms of performance, code coverage and handling.
  - added *mode* property: The class can derive exact solutions or estimate the kriging matrix for high performance gains
  - multiprocessing is supported now
  - the *solver* property can be used to choose from 3 different solver for the kriging matrix.
- [Variogram] deprecated *Variogram.compiled_model*. Use *Variogram.fitted_model* instead.
- [Variogram] added a new and much faster version of the parameterized model: *Variogram.fitted_model*

2.6.2 Version 0.2.5

- added *OrdinaryKriging* for using a *Variogram* to perform an interpolation.

2.6.3 Version 0.2.4

- added *SpaceTimeVariogram* for calculating dispersion functions depending on a space and a time lag.

2.6.4 Version 0.2.3

- **[severe bug]** A severe bug was in `Variogram.__vdiff_indexer` was found and fixed. The iterator was indexing the `Variogram._diff` array different from `Variogram.distance`. **This lead to wrong semivariance values for all versions > 0.1.8!**. Fixed now.
- [Variogram] added unit tests for parameter setting
- [Variogram] fixed `fit_sigma` setting of `'exp'`: changed the formula from $e^{\left(\frac{1}{x}\right)}$ to $1. - e^{\left(\frac{1}{x}\right)}$ in order to increase with distance and, thus, give less weight to distant lag classes during fitting.

2.6.5 Version 0.2.2

- added DirectionalVariogram class for direction-dependent variograms
- [Variogram] changed default values for *estimator* and *model* from function to string

2.6.6 Version 0.2.1

- added various unittests

2.6.7 Version 0.2.0

- completely rewritten Variogram class compared to v0.1.8