KramersMoyal

Release 0.4

Sep 07, 2021

Contents

`kramersmoyal` is a python package designed to obtain the Kramers—Moyal coefficients, or conditional moments, from stochastic data of any dimension. It employs kernel density estimations, instead of a histogram approach, to ensure better results for low number of points as well as allowing better fitting of the results.

CHAPTER 1

Installation

To install `kramersmoyal`, just use *pip*

```
pip install kramersmoyal
```

Then on your favourite editor just use

```
from kramersmoyal import km
```

From here you can simply call

```
import numpy as np

# Number of bins
bins = np.array([6000])

# Choose powers to calculate
powers = np.array([[1], [2]])

# And here x is your (1D, 2D, 3D) data
kmc, edge = km(x, bins = bins, powers = powers)
```

The library depends on `numpy` and `scipy`.

CHAPTER 2

A one-dimensional stochastic process

2.1 The theory

Take, for example, the well-documented one-dimension Ornstein—Uhlenbeck process, also known as Vašíček process. This process is governed by two main parameters: the mean-reverting parameter θ and the diffusion or volatility coefficient σ

$$\mathrm{d}y(t) = -\theta y(t)\mathrm{d}t + \sigma \mathrm{d}W(t)$$

which can be solved in various ways. For our purposes, recall that the drift coefficient, i.e., the first-order Kramers—Moyal coefficient, is given by $\mathcal{M}^{[1]}(y) = -\theta y$ and the second-order Kramers—Moyal coefficient is $\mathcal{M}^{[2]}(y) = \sigma^2/2$, i.e., the diffusion.

For this example let's take $\theta = 0.3$ and $\sigma = 0.1$, over a total time of 500 units, with a sampling of 1000 Hertz, and from the generated data series retrieve the two parameters, the drift $-\theta y(t)$ and diffusion σ.

2.2 Integrating an Ornstein—Uhlenbeck process

Here is a short code on generating a Ornstein—Uhlenbeck stochastic trajectory with a simple Euler–Maruyama integration method

```
# integration time and time sampling
t_final = 500
delta_t = 0.001

# The parameters theta and sigma
theta = 0.3
sigma = 0.1

# The time array of the trajectory
time = np.arange(0, t_final, delta_t)
```

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```
# Initialise the array y
y = np.zeros(time.size)

# Generate a Wiener process
dw = np.random.normal(loc = 0, scale = np.sqrt(delta_t), size = time.size)

# Integrate the process
for i in range(1,time.size):
    y[i] = y[i-1] - theta*y[i-1]*delta_t + sigma*dw[i]
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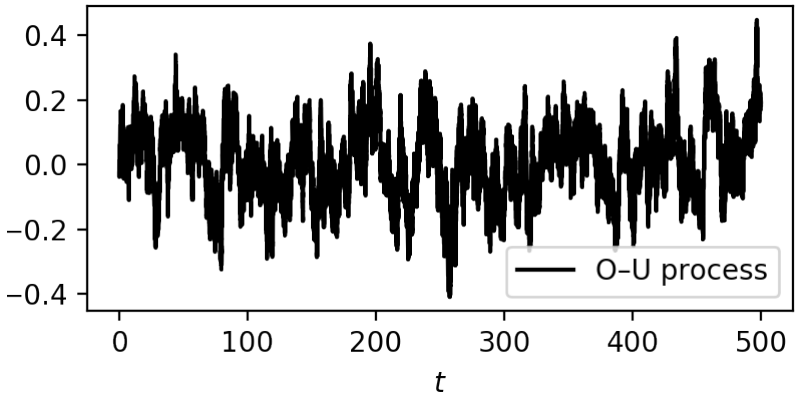
From here we have a plain example of an Ornstein—Uhlenbeck process, always drifting back to zero, due to the mean-reverting drift $-\theta y(t)$. The effect of the noise can be seen across the whole trajectory.



2.3 Using `kramersmoyal`

Take the timeseries $y(t)$ and let's study the Kramers—Moyal coefficients. For this let's look at the drift and diffusion coefficients of the process, i.e., the first and second Kramers—Moyal coefficients, with an `epanechnikov` kernel

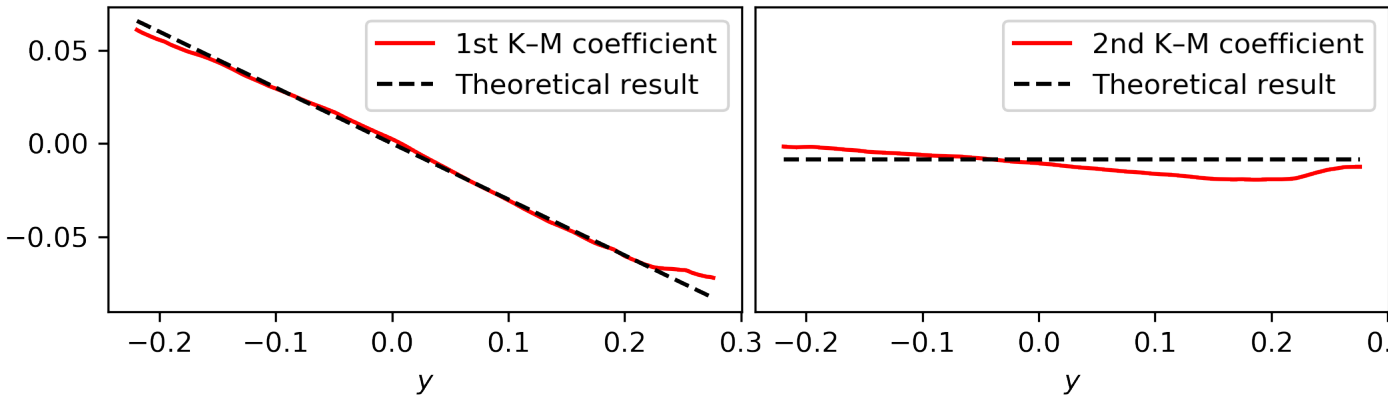
```
# Choose number of points of you target space
bins = np.array([5000])

# Choose powers to calculate
powers = np.array([[1], [2]])

# Choose your desired bandwith
bw = 0.15

# The kmc holds the results, where edges holds the binning space
kmc, edges = km(y, kernel = kernels.epanechnikov, bw = bw, bins = bins, powers =␣
↪powers)
```

This results in



Notice here that to obtain the Kramers—Moyal coefficients you need to divide `kmc` by the timestep `delta_t`. This normalisation stems from the Taylor-like approximation, i.e., the Kramers—Moyal expansion ($\delta t \to 0$).

CHAPTER 3

A two-dimensional diffusion process

3.1 Theory

A two-dimensional diffusion process is a stochastic process that comprises two $W(t)$ and allows for a mixing of these noise terms across its two dimensions.

$$\begin{pmatrix} \mathrm{d}y_1(t) \\ \mathrm{d}y_2(t) \end{pmatrix} = \begin{pmatrix} N_1(y) \\ N_2(y) \end{pmatrix} \mathrm{d}t + \begin{pmatrix} g_{1,1}(y) & g_{1,2}(y) \\ g_{2,1}(y) & g_{2,2}(y) \end{pmatrix} \begin{pmatrix} \mathrm{d}W_1 \\ \mathrm{d}W_2 \end{pmatrix}$$

with N the drift vector and g the diffusion matrix, which can be state dependent. We define, as the previous example, a process identical to the Ornstein—Uhlenbeck process, with

$$N = \begin{pmatrix} -N_1 y_1 \\ -N_2 y_2 \end{pmatrix}$$

and we take $N_1 = 2.0$ and $N_2 = 1.0$. For this particular case a more involved diffusion matrix g will be used. Let the matrix g be state-dependent, i.e., dependent of the actual values of y_1 and y_2 via

$$g = \begin{pmatrix} \frac{g_{1,1}}{1+e^{y_1^2}} & g_{1,2} \\ g_{2,1} & \frac{g_{2,2}}{1+e^{y_2^2}} \end{pmatrix}$$

and we will take $g_{1,1} = g_{2,2} = 0.5$ and $g_{1,2} = g_{2,1} = 0$.

3.2 Integrating a 2-dimensional process

Taking the above parameters and writing again an Euler–Maruyama integration method

```
# integration time and time sampling
t_final = 2000
delta_t = 0.001
```

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```
# Define the drift vector N
N = np.array([2.0, 1.0])

# Define the diffusion matrix g
g = np.array([[0.5, 0.0], [0.0, 0.5]])

# The time array of the trajectory
time = np.arange(0, t_final, delta_t)

# Initialise the array y
y = np.zeros([time.size, 2])

# Generate two Wiener processes with a scale of np.sqrt(delta_t)
dW = np.random.normal(loc = 0, scale = np.sqrt(delta_t), size = [time.size, 2])

# Integrate the process (takes about 20 secs)
for i in range(1, time.size):
    y[i,0] = y[i-1,0]  -  N[0] * y[i-1,0] * delta_t + g[0,0]/(1 + np.exp(y[i-1,
↪0]**2)) * dW[i,0]  +  g[0,1] * dW[i,1]
    y[i,1] = y[i-1,1]  -  N[1] * y[i-1,1] * delta_t + g[1,0] * dW[i,0]  +  g[1,1]/(1␣
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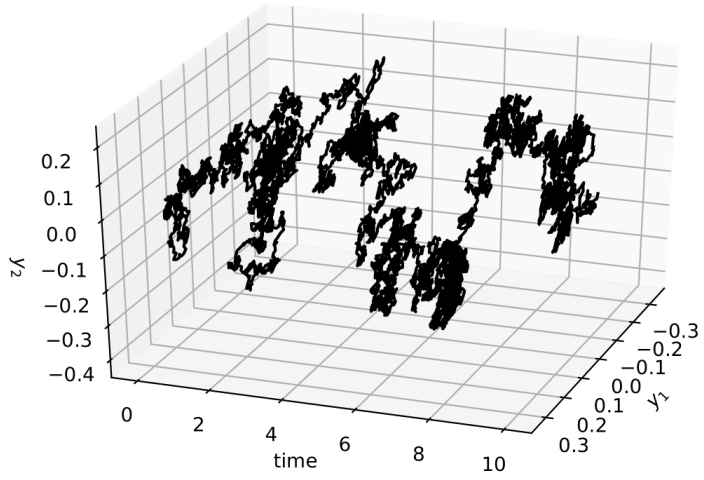
The stochastic trajectory in 2 dimensions for 10 time units (10000 data points)



3.3 Back to `kramersmoyal` and the Kramers—Moyal coefficients

First notice that all the results now will be two-dimensional surfaces, so we will need to plot them as such

```
# Choose the size of your target space in two dimensions
bins = np.array([300, 300])

# Introduce the desired orders to calculate, but in 2 dimensions
powers = np.array([[0,0], [1,0], [0,1], [1,1], [2,0], [0,2], [2,2]])
# insert into kmc:   0      1      2      3      4      5      6
```

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```
# Notice that the first entry in [,] is for the first dimension, the
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# Choose a desired bandwidth bw
bw = 0.1

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# The KM coefficients are stacked along the first dim of the
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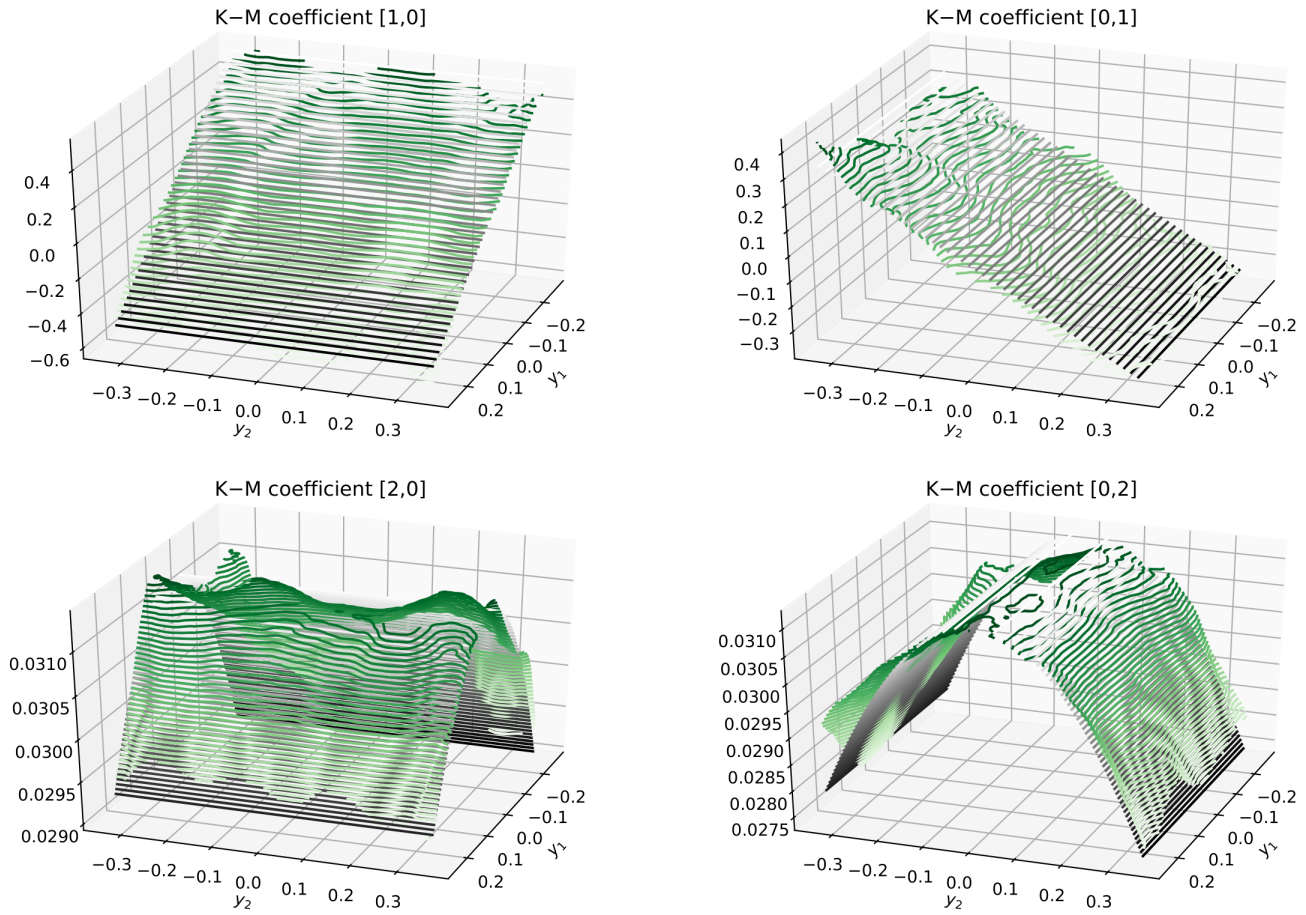
Now one can visualise the Kramers–Moyal coefficients (surfaces) in green and the respective theoretical surfaces in black. (Don't forget to normalise: `kmc / delta_t`).



CHAPTER 4

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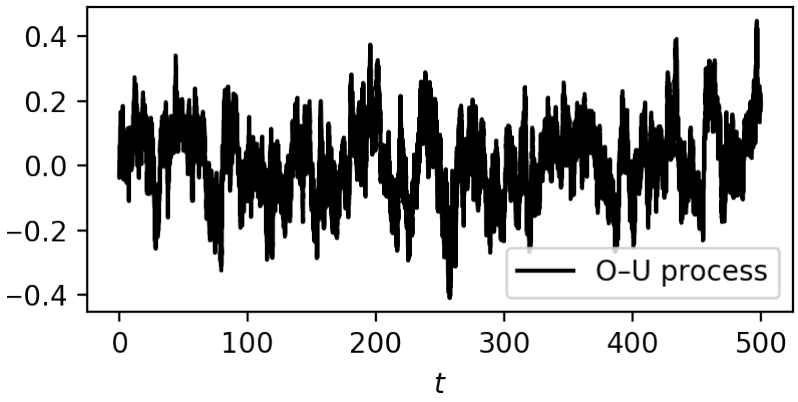

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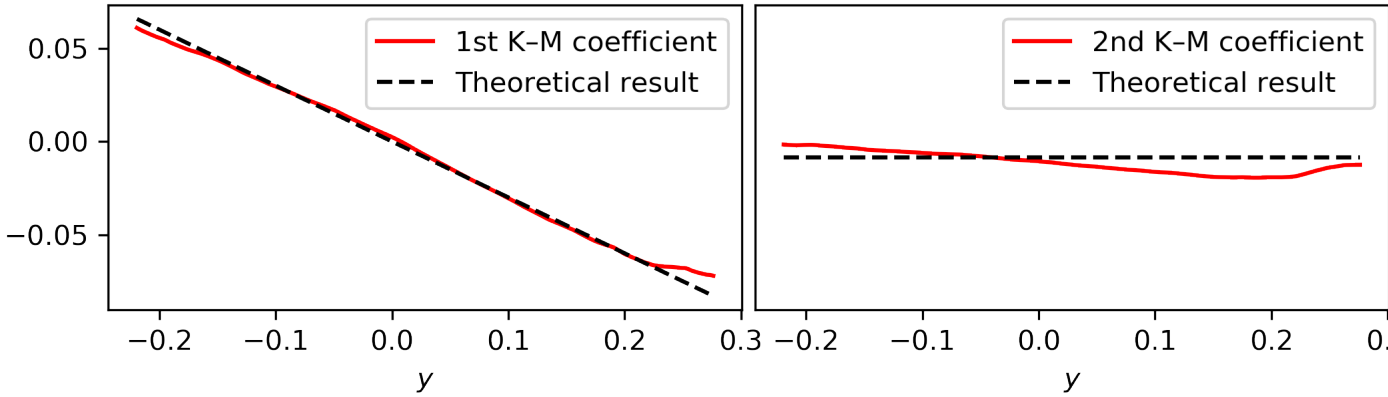

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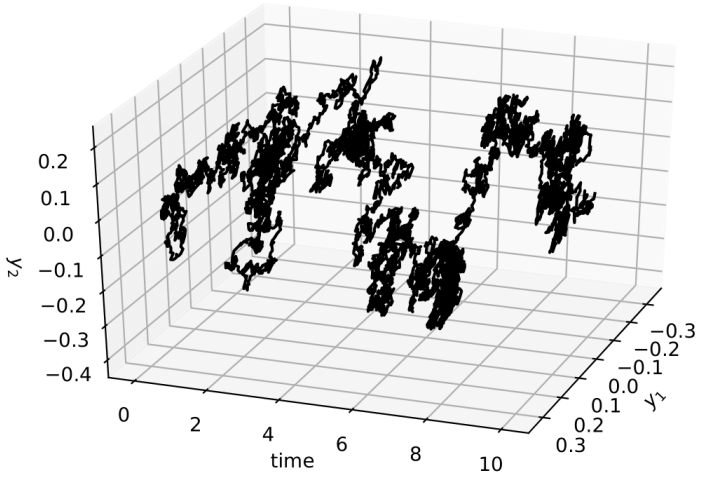

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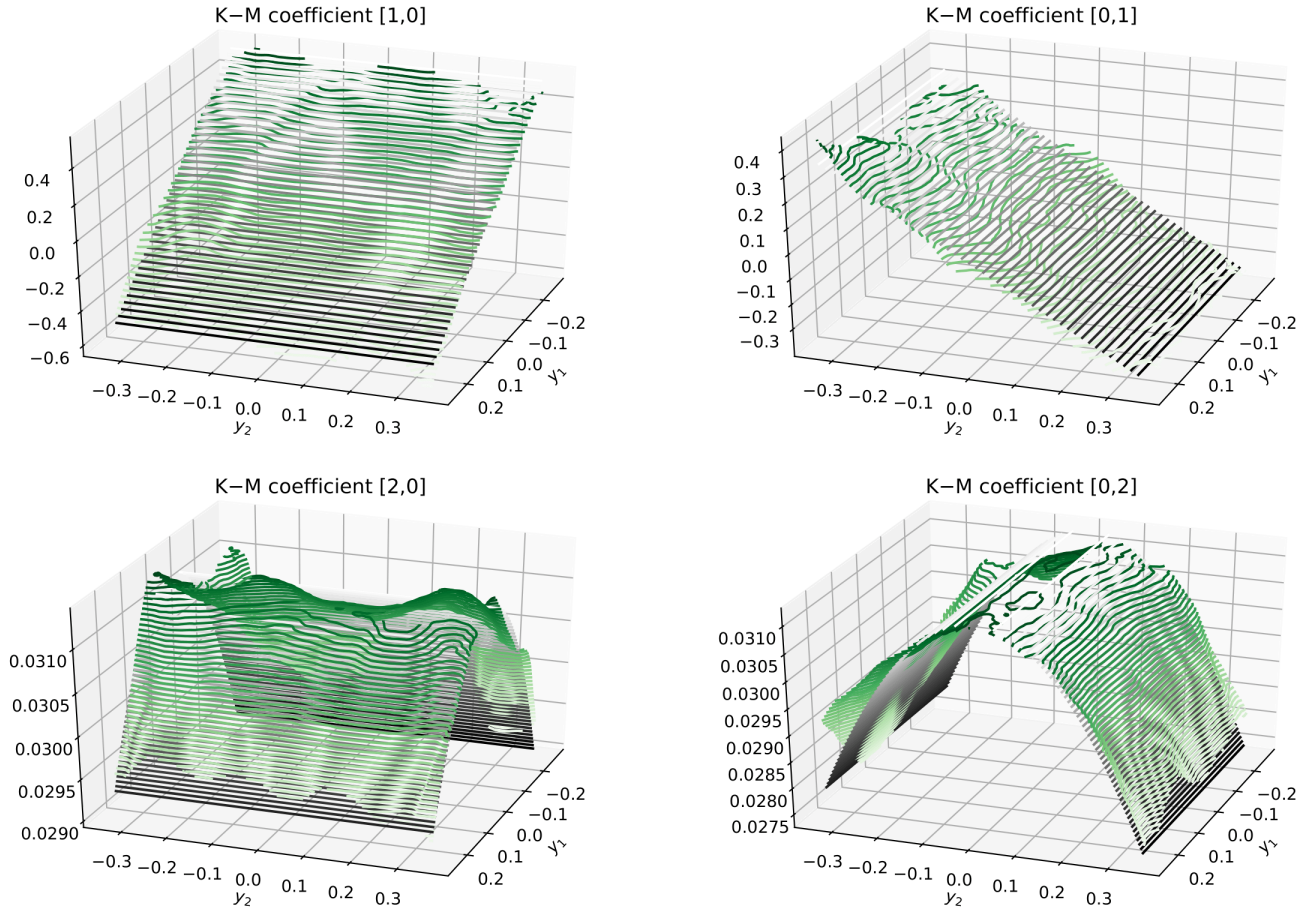

4.4 Functions

Documentation for all the functions in `kramersmoyal`.

4.4.1 Kramers—Moyal coefficients

`kramersmoyal.kmc.`**`km`**(*timeseries: numpy.ndarray*, *bins: numpy.ndarray*, *powers: numpy.ndarray*, *kernel: callable = <function epanechnikov>*, *bw: float = None*, *tol: float = 1e-10*, *conv_method: str = 'auto'*) → numpy.ndarray

Estimates the Kramers–Moyal coefficients from a timeseries using a kernel estimator method. `km` can calculate the Kramers–Moyal coefficients for a timeseries of any dimension, up to any desired power.

Parameters

- **`timeseries`** (*`np.ndarray`*) – The D-dimensional timeseries `(N, D)`. The timeseries of length `N` and dimensions `D`.
- **`bins`** (*`np.ndarray`*) – The number of bins for each dimension. This is the underlying space for the Kramers-Moyal coefficients. In 1-dimension a choice as

```
bins = np.array([6000])
```

is recommended. In 2-dimensions `bins = np.array([300,300])`

is recommended.

- **powers** (*np.ndarray*) – Powers for the operation of calculating the Kramers–Moyal coefficients, which need to match dimensions of the timeseries. In 1-dimension the first four Kramers-Moyal coefficients can be found via

  `powers = np.array([0],[1],[2],[3],[4]).`

  In 2 dimensions take into account each dimension, as

```
powers = np.array([0,0],[0,1],[1,0],[1,1],[0,2],[2,0],[2,2],
                  [0,3],[3,0],[3,3],[0,4],[4,0],[4,4])
```

kernel: callable (default epanechnikov) Kernel used to convolute with the Kramers-Moyal coefficients. To select for example a Gaussian kernel use

`kernel = kernels.gaussian`

bw: float (default None) Desired bandwidth of the kernel. A value of 1 occupies the full space of the bin space. Recommended are values `0.005 < bw < 0.5`.

tol: float (default 1e-10) Round to zero absolute values smaller than `tol`, after the convolutions.

conv_method: str (default auto) A string indicating which method to use to calculate the convolution. https://docs.scipy.org/doc/scipy/reference/generated/scipy.signal.convolve.html

Returns

- **kmc** (*np.ndarray*) – The calculated Kramers-Moyal coefficients in accordance to the time-series dimensions in (D,bins.shape) shape. To extract the selected orders of the kmc, use kmc[i,...], with i the order according to powers
- **edges** (*np.ndarray*) – The bin edges with shape (D,bins.shape) of the calculated Kramers-Moyal coefficients

4.4.2 Kernels

`kramersmoyal.kernels.`**`kernel`**(*kernel_func*)

Transforms a kernel function into a scaled kernel function (for a certain bandwidth `bw`)

Currently implemented kernels are: Epanechnikov, Gaussian, Uniform, Triangular, Quartic

For a good overview of various kernels see https://en.wikipedia.org/wiki/Kernel_(statistics)

`kramersmoyal.kernels.`**`epanechnikov`**(*x: numpy.ndarray*, *dims: int*) → numpy.ndarray

The Epanechnikov kernel in dimensions dims.

`kramersmoyal.kernels.`**`gaussian`**(*x: numpy.ndarray*, *dims: int*) → numpy.ndarray

Gaussian kernel in dimensions dims.

`kramersmoyal.kernels.`**`uniform`**(*x: numpy.ndarray*, *dims: int*) → numpy.ndarray

Uniform, or rectangular kernel in dimensions dims.

`kramersmoyal.kernels.`**`triagular`**(*x: numpy.ndarray*, *dims: int*) → numpy.ndarray

Triagular kernel in dimensions dims.

`kramersmoyal.kernels.`**`quartic`**(*x: numpy.ndarray*, *dims: int*) → numpy.ndarray

Quartic, or biweight kernel in dimensions dims.

4.4.3 Helping functions

Binning function

The `binning` function has no documentation

4.5 License

4.6 Contact

If you need help with something, find a bug, issue, or typo on the repository or in the code, you can contact me here: leonardo.rydin@gmail.com or open an issue on the GitHub repository.

CHAPTER 5

Literature

[1] Friedrich, R., Peinke, J., Sahimi, M., Tabar, M. R. R. *Approaching complexity by stochastic methods: From biological systems to turbulence,* [Phys. Rep. 506, 87–162 (2011)](https://doi.org/10.1016/j.physrep.2011.05.003).

The study of stochastic processes from a data-driven approach is grounded in extensive mathematical work. From the applied perspective there are several references to understand stochastic processes, the Fokker—Planck equations, and the Kramers—Moyal expansion

Tabar, M. R. R. (2019). *Analysis and Data-Based Reconstruction of Complex Nonlinear Dynamical Systems.* Springer, International Publishing

Risken, H. (1989). *The Fokker–Planck equation.* Springer, Berlin, Heidelberg.

Gardiner, C.W. (1985). *Handbook of Stochastic Methods.* Springer, Berlin.

An extensive review on the subject can be found here.

CHAPTER 6

Funding

Helmholtz Association Initiative *Energy System 2050 - A Contribution of the Research Field Energy* and the grant No. VH-NG-1025 and *STORM - Stochastics for Time-Space Risk Models* project of the Research Council of Norway (RCN) No. 274410.

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