KramersMoyal

Release 0.4

Contents

1	Installation	3	
2	A one-dimensional stochastic process 2.1 The theory	5 5 6	
3	A two-dimensional diffusion process 3.1 Theory	9 9 9 10	
4	Table of Content 4.1 Installation 4.2 A one-dimensional stochastic process 4.3 A two-dimensional diffusion process 4.4 Functions 4.5 License 4.6 Contact	13 13 15 18 20 21	
5	Literature	23	
6	Funding	25	
Bi	ibliography	27	
In	ndex	29	

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.

Contents 1

2 Contents

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.

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

$$dy(t) = -\theta y(t)dt + \sigma dW(t)$$

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)
```

(continues on next page)

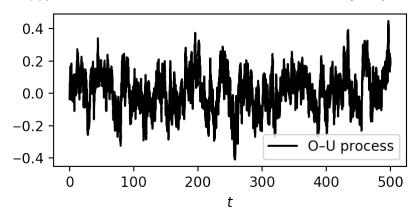
(continued from previous page)

```
# 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]
```

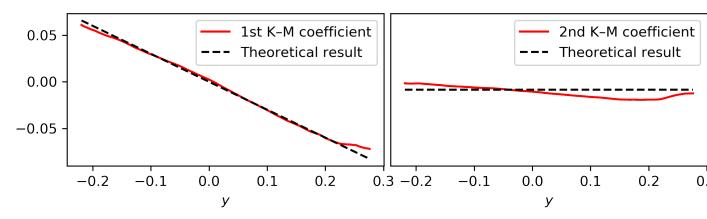
From here we have a plain example of an Ornstein—Uhlenbeck process, always drifting back to zero, due to the mean-reverting drift $-\theta y(t)$. The effect of the noise can be seen across the whole trajectory.



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 <code>epanechnikov</code> kernel

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
```

(continues on next page)

(continued from previous page)

```
# 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]])

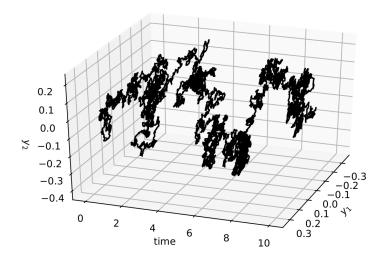
# The time array of the trajectory
time = np.arange(0, t_final, delta_t)

# 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_0) + np.exp(y[i-1,1]**2)) * dW[i,1]
```

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
```

(continues on next page)

(continued from previous page)

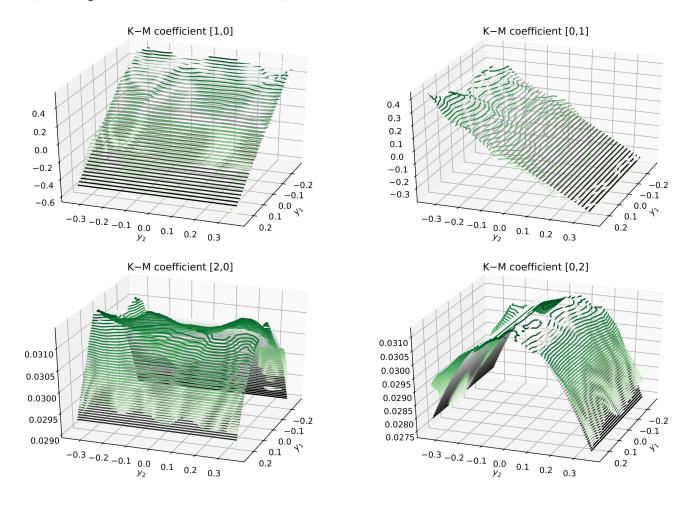
```
# Notice that the first entry in [,] is for the first dimension, the
# second for the second dimension...

# Choose a desired bandwidth bw
bw = 0.1

# Calculate the KramersMoyal coefficients
kmc, edges = km(y, bw = bw, bins = bins, powers = powers)

# The KM coefficients are stacked along the first dim of the
# kmc array, so kmc[1,...] is the first KM coefficient, kmc[2,...]
# is the second. These will be 2-dimensional matrices.
```

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

Table of Content

4.1 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.

4.2 A one-dimensional stochastic process

4.2.1 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

$$dy(t) = -\theta y(t)dt + \sigma dW(t)$$

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 .

4.2.2 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

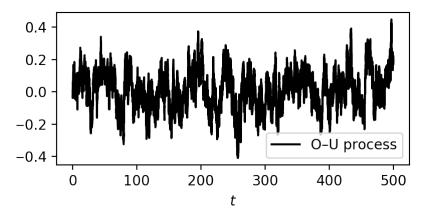
# The time array of the trajectory
time = np.arange(0, t_final, delta_t)

# 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]
```

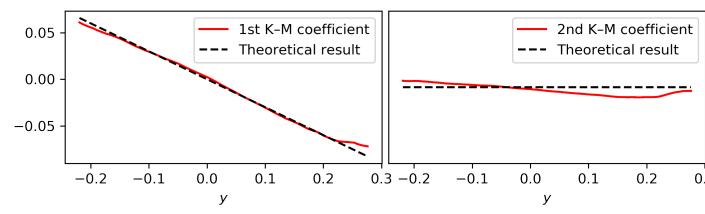
From here we have a plain example of an Ornstein—Uhlenbeck process, always drifting back to zero, due to the mean-reverting drift $-\theta y(t)$. The effect of the noise can be seen across the whole trajectory.



4.2.3 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

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 ($\delta t \to 0$).

4.3 A two-dimensional diffusion process

4.3.1 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

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

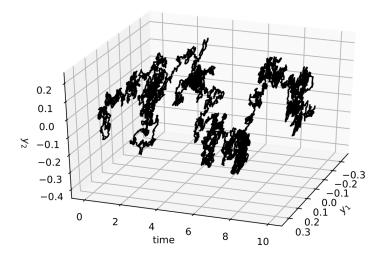
and we will take $g_{1,1} = g_{2,2} = 0.5$ and $g_{1,2} = g_{2,1} = 0$.

4.3.2 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
\# 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]))
\rightarrow0]**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_i)
\rightarrow+ np.exp(y[i-1,1]**2)) * dW[i,1]
```

The stochastic trajectory in 2 dimensions for 10 time units (10000 data points)



4.3.3 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

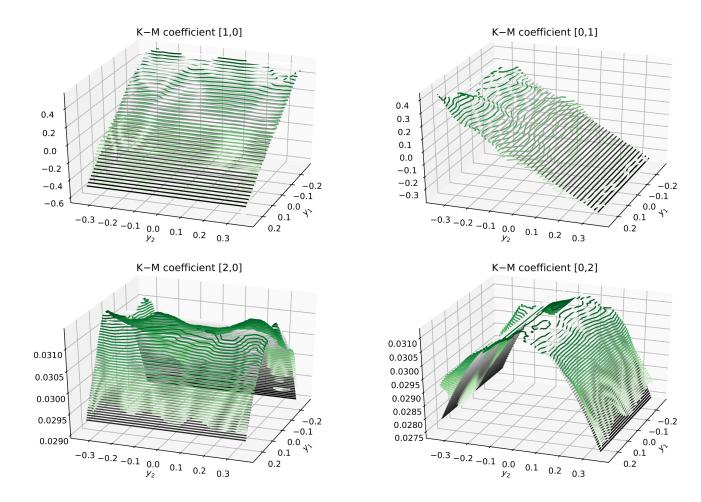
# Notice that the first entry in [,] is for the first dimension, the
# second for the second dimension...

# Choose a desired bandwidth bw
bw = 0.1

# Calculate the KramersMoyal coefficients
kmc, edges = km(y, bw = bw, bins = bins, powers = powers)

# The KM coefficients are stacked along the first dim of the
# kmc array, so kmc[1,...] is the first KM coefficient, kmc[2,...]
# is the second. These will be 2-dimensional matrices.
```

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).



4.4 Functions

Documentation for all the functions in kramersmoyal.

4.4.1 Kramers—Moyal coefficients

kramersmoyal.kmc.km(timeseries: numpy.ndarray, bins: str = 'default', powers: int = 4, kernel: callable = <function epanechnikov>, bw: float = None, tol: float = 1e-10, conv_method: str = 'auto', center_edges: bool = True, full: bool = False) -> (<class 'numpy.ndarray'>, <class '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** (int or list or np.ndarray or string (default *default*)) The number of bins. This is the underlying space for the Kramers–Moyal coefficients to be estimated. If desired, bins along each dimension can be given as monotonically increasing bin edges (tuple or list), e.g.,

- in 1-D, (np.linspace(lower, upper, length),);
- in 2-D, '(np.linspace(lower_x, upper_x, length_x), np.linspace(lower_y, upper_y, length_y))',

with desired *lower* and *upper* ranges (in each dimension). If default, the bin numbers for different dimensions are:

- 1-D, 5000;
- 2-D, 100×100;
- 3-D, 25×25×25.

The bumber of bins along each dimension can be specified, e.g.,

- 2-D, [125, 75],
- 3-D, [100, 80, 120].

If bins is int, or a list or np.array of dimension 1, and the timeseries dimension is D, then int(bins**(1/D)).

- **powers** (int or list or tuple or np.ndarray (default 4)) Powers for the operation of calculating the Kramers–Moyal coefficients. Default is the largest power used, e.g., if 4, then (0, 1, 2, 3, 4). They can be specified, matching the dimensions of the timeseries. E.g., in 1-dimension the first four Kramers–Moyal coefficients can be given as *powers*=(0, 1, 2, 3, 4), which is the same as *powers*=4. Setting *powers*=p for higher dimensions will results in all possible combinations up to the desired power 'p', e.g.
 - 2-D, powers=2 results in

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

Set *full=True* to output *powers*. The order that they appear dictactes the order in the output *kmc*

• **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. Set *full=True* to output bw.
- 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
- **center_edges** (bool (default True)) Whether to return the bin centers or the bin edges (since for n bins there are n + 1 edges).
- **full** (bool (default *False*)) Outputs bandwidth *bw* and powers *powers*.

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.

4.4. Functions

- edges (*np.ndarray*) The bin edges with shape (*D*, *bins.shape*) of the estimated Kramers–Moyal coefficients.
- (..., bw, powers) (tuple) This is only returned if full=True:
 - The bandwidth bw,
 - An array of the *powers*.

References

drift and diffusion coefficients of stochastic processes." Physics Letters A 373(39), 3507–3512, 2009.

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) \rightarrow numpy.ndarray The Epanechnikov kernel in dimensions dims.
- kramersmoyal.kernels.gaussian (x: numpy.ndarray, dims: int) \rightarrow numpy.ndarray Gaussian kernel in dimensions dims.
- kramersmoyal.kernels.uniform (x: numpy.ndarray, dims: int) \rightarrow numpy.ndarray Uniform, or rectangular kernel in dimensions dims.
- kramersmoyal.kernels.triagular (x: numpy.ndarray, dims: int) \rightarrow numpy.ndarray Triagular kernel in dimensions dims.
- $\label{eq:continuous} \textbf{Rernels.quartic} \ (\textit{x: numpy.ndarray}, \textit{dims: int}) \ \rightarrow \textbf{numpy.ndarray} \\ \textbf{Quartic, or biweight kernel in dimensions dims.}$

4.4.3 Helping functions

Binning function

The binning function has no documentation

4.5 License

MIT License

Copyright (c) 2019–2023 Leonardo Rydin Gorjão

Permission is hereby granted, free of charge, to any person obtaining a copy of this software and associated documentation files (the "Software"), to deal in the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the Software, and to permit persons to whom the Software is furnished to do so, subject to the following conditions:

The above copyright notice and this permission notice shall be included in all copies or substantial portions of the Software.

THE SOFTWARE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE AND NONINFRINGEMENT. IN NO EVENT SHALL THE AUTHORS OR COPYRIGHT HOLDERS BE LIABLE FOR ANY CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.

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.

4.6. Contact 21

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.

CHAP	TED	h
\cup \square \land \vdash	'I ER	U

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.

26 Chapter 6. Funding

	Bibliography

[Lamouroux2009] D. Lamouroux and K. Lehnertz, "Kernel-based regression of

28 Bibliography

Index

```
E
epanechnikov() (in module kramersmoyal.kernels), 20

G
gaussian() (in module kramersmoyal.kernels), 20

K
kernel() (in module kramersmoyal.kernels), 20
km() (in module kramersmoyal.kmc), 18
kramersmoyal.kernels (module), 20
kramersmoyal.kmc (module), 18

Q
quartic() (in module kramersmoyal.kernels), 20

T
triagular() (in module kramersmoyal.kernels), 20

U
uniform() (in module kramersmoyal.kernels), 20
```