QuadratiK

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CONTENTS

1	Intro	duction											1
	1.1	Fundi	ng Informa	ation		 	 	 		 	 		1
	1.2	Autho	rs			 	 	 		 	 		1
	1.3	Refere	ences			 	 	 		 	 		1
2	Getti	ing star	rted										3
	2.1					 	 	 		 	 		3
		2.1.1	_	tion									3
			2.1.1.1	Which Python?									3
			2.1.1.2	Install using pip									3
			2.1.1.3	Dependencies .									3
			2.1.1.4	Testing									4
							 					 -	
3		Referen											5
	3.1												5
		3.1.1		Test									5
			3.1.1.1	KernelTest									5
			3.1.1.2										9
		3.1.2		Kernel Test									11
			3.1.2.1	PoissonKernelTe									11
		3.1.3	_	al Clustering									14
			3.1.3.1	PKBC									14
			3.1.3.2	PKBD									17
		3.1.4		terface									19
			3.1.4.1	UI									19
		3.1.5		s									20
			3.1.5.1	load_wireless_da									20
		3.1.6	Tools										22
			3.1.6.1	sample_hypersph	nere	 	 	 		 	 	 •	22
			3.1.6.2	stats									23
			3.1.6.3	qq_plot									23
			3.1.6.4	sphere3d									24
			3.1.6.5	plot_clusters_2d		 	 	 	• •	 	 	 •	25
4	User	Guide											26
	4.1	User (Guide			 	 	 		 	 		26
		4.1.1											26
			4.1.1.1	Wireless Indoor									26
		4.1.2	Usage I										27
			4.1.2.1	QuadratiK Usage									27
				-									

Python Module Index	39
Index	40

CHAPTER

ONE

INTRODUCTION

The QuadratiK package is implemented in both \mathbf{R} and \mathbf{Python} , providing a comprehensive set of goodness-of-fit tests and a clustering technique using kernel-based quadratic distances. This framework aims to bridge the gap between the statistical and machine learning literatures. It includes:

- Goodness-of-Fit Tests: The software implements one, two, and k-sample tests for goodness of fit, offering an efficient and mathematically sound way to assess the fit of probability distributions. Expanded capabilities include supporting tests for uniformity on the d-dimensional Sphere based on Poisson kernel densities.
- Clustering Algorithm for Spherical Data: the package incorporates a unique clustering algorithm specifically tailored for spherical data. This algorithm leverages a mixture of Poisson-kernel-based densities on the sphere, enabling effective clustering of spherical data or data that has been spherically transformed. This facilitates the uncovering of underlying patterns and relationships in the data.
- Additional Features: Alongside these functionalities, the software includes additional graphical functions, aiding users in validating cluster results as well as visualizing and representing clustering results. This enhances the interpretability and usability of the analysis.

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1.3 References

Saraceno G., Markatou M., Mukhopadhyay R., Golzy M. (2023). Goodness of- fit and clustering of spherical data: The QuadratiK package in R and Python. Technical Report, Department of Biostatistics, University at Buffalo.

Ding Y., Markatou M., Saraceno G. (2023). "Poisson Kernel-Based Tests for Uniformity on the d-Dimensional Sphere." Statistica Sinica. doi: doi:10.5705/ss.202022.0347.

Golzy M. & Markatou M. (2020) Poisson Kernel-Based Clustering on the Sphere: Convergence Properties, Identifiability, and a Method of Sampling, Journal of Computational and Graphical Statistics, 29:4, 758-770, DOI: 10.1080/10618600.2020.1740713.

Markatou M, Saraceno G, Chen Y (2023). "Two- and k-Sample Tests Based on Quadratic Distances." Manuscript, (Department of Biostatistics, University at Buffalo).

1.3. References 2

CHAPTER

TWO

GETTING STARTED

2.1 Getting Started

2.1.1 Installation

2.1.1.1 Which Python?

You'll need Python 3.9 (except 3.9.7) or greater.

2.1.1.2 Install using pip

pip install /path/to/package

2.1.1.3 Dependencies

QuadratiK requires the following (arranged alphabetically):

- asyncio (>=3.4)
- matplotlib (>=3.8.2)
- nest-asyncio (>=1.5)
- numpy (>= 1.26.2)
- pandas (>= 2.1.3)
- plotly (>=5.15.0)
- scikit-learn (>= 1.3)
- scipy (>= 1.11)
- streamlit (>=1.29.0)
- tabulate (>= 0.8)

2.1.1.4 **Testing**

QuadratiK uses the Python pytest package. To install pytest, please go here. To run the tests using pytest, please follow these instructions. Navigate to the tests folder to run the tests.

2.1. Getting Started

CHAPTER

THREE

API REFERENCE

3.1 API Reference

3.1.1 Kernel Test

KernelTest([h, method, num_iter, b,])	Class for performing the kernel-based quadratic distance Goodness-of-fit tests using the Gaussian kernel with tun- ing parameter h.
select_h(x[, y, alternative, method, b,])	This function computes the kernel bandwidth of the Gaussian kernel for the one sample, two-sample and ksample kernel-based quadratic distance (KBQD) tests.

3.1.1.1 KernelTest

Class for performing the kernel-based quadratic distance goodness-of-fit tests using the Gaussian kernel with tuning parameter h. Depending on the input y the function performs the test of multivariate normality, the non-parametric two-sample tests or the k-sample tests.

Parameters

h

[float, optional] Bandwidth for the kernel function.

method

[str, optional] The method used for critical value estimation ("subsampling", "bootstrap", or "permutation").

num_iter

[int, optional] The number of iterations to use for critical value estimation. Defaults to 150.

b

[float, optional] The size of the subsamples used in the subsampling algorithm. Defaults to 0.9.

quantile

[float, optional] The quantile to use for critical value estimation. Defaults to 0.95.

mu hat

[numpy.ndarray, optional] Mean vector for the reference distribution. Defaults to None.

sigma_hat

[numpy.ndarray, optional] Covariance matrix of the reference distribution. Defaults to None.

alternative

[str, optional] String indicating the type of alternative to be used for calculating "h" by the tuning parameter selection algorithm when h is not provided. Defaults to 'None'

k_threshold

[int, optional] Maximum number of groups allowed. Defaults to 10. Change in case of more than 10 groups.

random_state

[int, None, optional.] Seed for random number generation. Defaults to None

n_jobs

[int, optional.] n_jobs specifies the maximum number of concurrently running workers. If 1 is given, no joblib parallelism is used at all, which is useful for debugging. For more information on joblib n_jobs refer to - https://joblib.readthedocs.io/en/latest/generated/joblib.Parallel.html. Defaults to 8.

Attributes

test_type_

[str] The type of test performed on the data

execution_time

[float] Time taken for the test method to execute

h0_rejected_

[boolean] Whether the null hypothesis is rejected (True) or not (False)

test_statistic_

[float] Test statistic of the perfomed test type

cv

[float] Critical value

cv method

[str] Critical value method used for performing the test

References

Markatou M., Saraceno G., Chen Y (2023). "Two- and k-Sample Tests Based on Quadratic Distances." Manuscript, (Department of Biostatistics, University at Buffalo)

Lindsay BG, Markatou M. & Ray S. (2014) Kernels, Degrees of Freedom, and Power Properties of Quadratic Distance Goodness-of-Fit Tests, Journal of the American Statistical Association, 109:505, 395-410, DOI: 10.1080/01621459.2013.836972

Examples

```
>>> # Example for normality test
>>> import numpy as np
>>> from QuadratiK.kernel_test import KernelTest
>>> np.random.seed(42)
>>> data = np.random.randn(100,5)
>>> normality_test = KernelTest(h=0.4, centering_type="param",random_state=42).
→test(data)
>>> print("Test : {}".format(normality_test.test_type_))
>>> print("Execution time: {:.3f}".format(normality_test.execution_time))
>>> print("H0 is Rejected : {}".format(normality_test.h0_rejected_))
>>> print("Test Statistic : {}".format(normality_test.test_statistic_))
>>> print("Critical Value (CV) : {}".format(normality_test.cv_))
>>> print("CV Method : {}".format(normality_test.cv_method_))
>>> print("Selected tuning parameter : {}".format(normality_test.h))
... Test : Kernel-based quadratic distance Normality test
... Execution time: 0.096
... HO is Rejected : False
... Test Statistic : -8.588873037044384e-05
... Critical Value (CV) : 0.0004464111809800183
... CV Method : Empirical
... Selected tuning parameter: 0.4
```

```
>>> # Example for two sample test
>>> import numpy as np
>>> from QuadratiK.kernel_test import KernelTest
>>> np.random.seed(42)
\rightarrow > X = np.random.randn(100,5)
>>> np.random.seed(42)
\rightarrow > Y = np.random.randn(100,5)
>>> two_sample_test = KernelTest(h=0.4, centering_type="param").test(X,Y)
>>> print("Test : {}".format(two_sample_test.test_type_))
>>> print("Execution time: {:.3f}".format(two_sample_test.execution_time))
>>> print("H0 is Rejected : {}".format(two_sample_test.h0_rejected_))
>>> print("Test Statistic : {}".format(two_sample_test.test_statistic_))
>>> print("Critical Value (CV) : {}".format(two_sample_test.cv_))
>>> print("CV Method : {}".format(two_sample_test.cv_method_))
>>> print("Selected tuning parameter : {}".format(two_sample_test.h))
... Test : Kernel-based quadratic distance two-sample test
... Execution time: 0.092
... HO is Rejected : False
... Test Statistic : -0.019707895277270022
... Critical Value (CV) : 0.003842482597612725
... CV Method : subsampling
... Selected tuning parameter : 0.4
```

Methods

KernelTest.stats()	Function to generate descriptive statistics per variable (and per group if available).
<pre>KernelTest.summary([print_fmt])</pre>	Summary function generates a table for the kernel test results and the summary statistics.
KernelTest.test(x[,y])	Function to perform the kernel-based quadratic distance tests using the Gaussian kernel with bandwidth parameter h.

KernelTest.stats()

Function to generate descriptive statistics per variable (and per group if available).

Returns

summary_stats_df

[pandas.DataFrame] Dataframe of descriptive statistics

KernelTest.summary(print_fmt='simple_grid')

Summary function generates a table for the kernel test results and the summary statistics.

Parameters

print_fmt

[str, optional.] Used for printing the output in the desired format. Defaults to "simple_grid". Supports all available options in tabulate, see here: https://pypi.org/project/tabulate/

Returns

summary

[str] A string formatted in the desired output format with the kernel test results and summary statistics.

KernelTest.test(x, y=None)

Function to perform the kernel-based quadratic distance tests using the Gaussian kernel with bandwidth parameter h. Depending on the shape of the y, the function performs the tests of multivariate normality, the non-parametric two-sample tests or the k-sample tests.

Parameters

x [numpy.ndarray or pandas.DataFrame.] A numeric array of data values.

y [numpy.ndarray or pandas.DataFrame, optional] A numeric array data values (for two-sample test) and a 1D array of class labels (for k-sample test). Defaults to None.

Returns

self

[object] Fitted estimator

3.1.1.2 select h

```
QuadratiK.kernel_test.select_h(x, y=None, alternative='location', method='subsampling', b=0.8, num_iter=150, delta_dim=1, delta=None, h_values=None, n_rep=50, n_jobs=8, quantile=0.95, k_threshold=10, power_plot=False, random_state=None)
```

This function computes the kernel bandwidth of the Gaussian kernel for the one sample, two-sample and k-sample kernel-based quadratic distance (KBQD) tests.

The function performs the selection of the optimal value for the tuning parameter h of the normal kernel function, for the two-sample and k-sample KBQD tests. It performs a small simulation study, generating samples according to the family of alternative specified, for the chosen values of h_values and delta.

Parameters

x [numpy.ndarray or pandas.DataFrame] Data set of observations from X

y [numpy.ndarray or pandas.DataFrame, optional] Data set of observations from Y for two sample test or set of labels in case of k-sample test

alternative

[str, optional] Family of alternative chosen for selecting h, must be one of "location", "scale" and "skewness". Defaults to "location"

method

[str, optional.] The method used for critical value estimation, must be one of "subsampling", "bootstrap", or "permutation". Defaults to "subsampling".

 ${\bf b}$ [float, optional.] The size of the subsamples used in the subsampling algorithm. Defaults to 0.8.

num_iter

[int, optional.] The number of iterations to use for critical value estimation. Defaults to 150.

delta dim

[int, numpy.ndarray, optional.] Array of coefficient of alternative with respect to each dimension. Defaults to 1.

delta

[numpy.ndarray, optional.] Array of parameter values indicating chosen alternatives. Defaults to None.

h values

[numpy.ndarray, optional.] Values of the tuning parameter used for the selection. Defaults to None.

n_rep

[int, optional. Defaults to 50.] Number of bootstrap replications

n_jobs

[int, optional.] n_jobs specifies the maximum number of concurrently running workers. If 1 is given, no joblib parallelism is used at all, which is useful for debugging. For more information on joblib n_jobs refer to - https://joblib.readthedocs.io/en/latest/generated/joblib.Parallel.html. Defaults to 8.

quantile

[float, optional.] Quantile to use for critical value estimation. Defaults to 0.95.

k threshold

[int.] Maximum number of groups allowed. Defaults to 10.

power_plot

[boolean, optional.] If True, plot is displayed the plot of power for values in h_values and delta. Defaults to False.

random state

[int, None, optional.] Seed for random number generation. Defaults to None

Returns

h

[float] The selected value of tuning parameter h

h vs Power table

[pandas.DataFrame] A table containing the h, delta and corresponding powers

References

Markatou M., Saraceno G., Chen Y. (2023). "Two- and k-Sample Tests Based on Quadratic Distances." Manuscript, (Department of Biostatistics, University at Buffalo)

Examples

```
>>> import numpy as np
>>> from QuadratiK.kernel_test import select_h
>>> np.random.seed(42)
>>> X = np.random.randn(200, 2)
>>> np.random.seed(42)
>>> y = np.random.randint(0, 2, 200)
>>> h_selected, all_values, power_plot = select_h(
... X, y, alternative='location', power_plot=True, random_state=42)

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```

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```
>>> print("Selected h is: ", h_selected)
... Selected h is: 1.2
```

3.1.2 Poisson Kernel Test

PoissonKernelTest([rho, num_iter, quantile, ...]) Class for Poisson kernel-based quadratic distance test of Uniformity on the Sphere

3.1.2.1 PoissonKernelTest

Class for Poisson kernel-based quadratic distance test of Uniformity on the Sphere

Parameters

rho

[float] The value of concentration parameter used for the Poisson kernel function.

num_iter

[int, optional] Number of iterations for critical value estimation of U-statistic.

anantile

[float, optional] The quantile to use for critical value estimation

random state

[int, None, optional.] Seed for random number generation. Defaults to None

n_jobs

[int, optional.] n_jobs specifies the maximum number of concurrently running workers. If 1 is given, no joblib parallelism is used at all, which is useful for debugging. For more information on joblib n_jobs refer to - https://joblib.readthedocs.io/en/latest/generated/joblib.Parallel.html. Defaults to 8.

Attributes

test_type_

[str] The type of test performed on the data

execution time

[float] Time taken for the test method to execute

u_statistic_h0_

[boolean] A logical value indicating whether or not the null hypothesis is rejected according to Un

u statistic un

[float] The value of the U-statistic.

u statistic cv

[float] The empirical critical value for Un

```
v_statistic_h0_
    [boolean] A logical value indicating whether or not the null hypothesis is rejected according to Vn.

v_statistic_vn_
    [float] The value of the V-statistic.

v_statistic_cv_
    [float] The critical value for Vn computed following the asymptotic distribution.
```

References

Ding Y., Markatou M., Saraceno G. (2023). "Poisson Kernel-Based Tests for Uniformity on the d-Dimensional Sphere." Statistica Sinica. doi: doi:10.5705/ss.202022.0347

Examples

```
>>> from QuadratiK.tools import sample_hypersphere
>>> from QuadratiK.poisson_kernel_test import PoissonKernelTest
>>> np.random.seed(42)
>>> X = sample_hypersphere(100,3, random_state=42)
>>> unif_test = PoissonKernelTest(rho = 0.7, random_state=42).test(X)
>>> print("Execution time: {:.3f} seconds".format(unif_test.execution_time))
>>> print("U Statistic Results")
>>> print("H0 is rejected : {}".format(unif_test.u_statistic_h0_))
>>> print("Un Statistic : {}".format(unif_test.u_statistic_un_))
>>> print("Critical Value : {}".format(unif_test.u_statistic_cv_))
>>> print("V Statistic Results")
>>> print("H0 is rejected : {}".format(unif_test.v_statistic_h0_))
>>> print("Vn Statistic : {}".format(unif_test.v_statistic_vn_))
>>> print("Critical Value : {}".format(unif_test.v_statistic_cv_))
... Execution time: 0.181 seconds
... U Statistic Results
... H0 is rejected : False
... Un Statistic : 1.6156682048968174
... Critical Value : 0.06155875299050079
... V Statistic Results
... HO is rejected : False
... Vn Statistic : 22.83255917641962
... Critical Value : 23.229486935225513
```

Methods

PoissonKernelTest.stats()	Function to generate descriptive statistics.
<pre>PoissonKernelTest.summary([print_fmt])</pre>	Summary function generates a table for the poisson kernel test results and the summary statistics.
PoissonKernelTest.test(x)	Performs the Poisson kernel-based quadratic distance Goodness-of-fit tests for Uniformity for spherical data using the Poisson kernel with concentration parameter rho

PoissonKernelTest.stats()

Function to generate descriptive statistics.

Returns

summary_stats_df

[pandas.DataFrame] Dataframe of descriptive statistics

PoissonKernelTest.summary(print_fmt='simple_grid')

Summary function generates a table for the poisson kernel test results and the summary statistics.

Parameters

print_fmt

[str, optional.] Used for printing the output in the desired format. Supports all available options in tabulate, see here: https://pypi.org/project/tabulate/. Defaults to "simple_grid".

Returns

summary

[str] A string formatted in the desired output format with the kernel test results and summary statistics.

PoissonKernelTest.test(x)

Performs the Poisson kernel-based quadratic distance Goodness-of-fit tests for Uniformity for spherical data using the Poisson kernel with concentration parameter $\it rho$

Parameters

X

[numpy.ndarray, pandas.DataFrame] a numeric d-dim matrix of data points on the Sphere $S^{(d-1)}$.

Returns

self

[object] Fitted estimator

3.1.3 Spherical Clustering

<pre>PKBC([num_clust, max_iter, stopping_rule,])</pre>	Poisson kernel-based clustering on the Sphere.
PKBD()	Class for estimating density and generating samples of
	Poisson-kernel based distribution (PKBD).

3.1.3.1 PKBC

Poisson kernel-based clustering on the sphere. The class performs the Poisson kernel-based clustering algorithm on the sphere based on the Poisson kernel-based densities. It estimates the parameter of a mixture of Poisson kernel-based densities. The obtained estimates are used for assigning final memberships, identifying the data points.

Parameters

num clust

[int] Number of clusters.

max iter

[int] Maximum number of iterations before a run is terminated.

stopping_rule

[str, optional] String describing the stopping rule to be used within each run. Currently must be either 'max', 'membership', or 'loglik'.

init_method

[str, optional] String describing the initialization method to be used. Currently must be 'sample-Data'.

num init

[int, optional] Number of initializations.

tol

[float.] Constant defining threshold by which log likelihood must change to continue iterations, if applicable. Defaults to 1e-7.

random state

[int, None, optional.] Seed for random number generation. Defaults to None

n jobs

[int] Used only for computing the WCSS efficiently. n_jobs specifies the maximum number of concurrently running workers. If 1 is given, no joblib parallelism is used at all, which is useful for debugging. For more information on joblib n_jobs refer to - https://joblib.readthedocs.io/en/latest/generated/joblib.Parallel.html. Defaults to 4.

Attributes

alpha

[numpy.ndarray of shape (n_clusters,)] Estimated mixing proportions

labels

[numpy.ndarray of shape (n_samples,)] Final cluster membership assigned by the algorithm to each observation

log_lik_vec

[numpy.ndarray of shape (num_init,)] Array of log-likelihood values for each initialization

loklik_

[float] Maximum value of the log-likelihood function

mu

[numpy.ndarray of shape (n_clusters, n_features)] Estimated centroids

num_iter_per_run

[numpy.ndarray of shape (num_init,)] Number of E-M iterations per run

post_probs_

[numpy.ndarray of shape (n_samples, n_features)] Posterior probabilities of each observation for the indicated clusters

rho

[numpy.ndarray of shape (n_clusters,)] Estimated concentration parameters rho

euclidean wcss

[float] Values of within-cluster sum of squares computed with Euclidean distance.

cosine_wcss_

[float] Values of within-cluster sum of squares computed with cosine similarity.

References

Golzy M. & Markatou M. (2020) Poisson Kernel-Based Clustering on the Sphere: Convergence Properties, Identifiability, and a Method of Sampling, Journal of Computational and Graphical Statistics, 29:4, 758-770, DOI: 10.1080/10618600.2020.1740713.

Examples

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Methods

PKBC.fit(dat)	Performs Poisson Kernel-based Clustering.
PKBC.stats()	Function to generate descriptive statistics per variable
	(and per group if available).
PKBC.validation([y_true])	Computes validation metrics such as ARI, Macro Precision and Macro Recall when true labels are provided.

PKBC.fit(dat)

Performs Poisson Kernel-based Clustering.

Parameters

dat

[numpy.ndarray, pandas.DataFrame] A numeric array of data values.

Returns

self

[object] Fitted estimator

PKBC.stats()

Function to generate descriptive statistics per variable (and per group if available).

Returns

summary_stats_df

[pandas.DataFrame] Dataframe of descriptive statistics

PKBC.validation(y_true=None)

Computes validation metrics such as ARI, Macro Precision and Macro Recall when true labels are provided.

Parameters

y_true

[numpy.ndarray.] Array of true memberships to clusters, Defaults to None.

Returns

validation metrics

[tuple] The tuple consists of the following:

Adjusted Rand Index

[float (returned only when y_true is provided)] Adjusted Rand Index computed between the true and predicted cluster memberships.

• Macro Precision

[float (returned only when y_true is provided)] Macro Precision computed between the true and predicted cluster memberships.

Macro Recall

[float (returned only when y_true is provided)] Macro Recall computed between the true and predicted cluster memberships.

• Average Silhouette Score

[float] Mean Silhouette Coefficient of all samples.

References

Rousseeuw, P.J. (1987) Silhouettes: A graphical aid to the interpretation and validation of cluster analysis. Journal of Computational and Applied Mathematics, 20, 53–65.

Notes

We have taken a naive approach to map the predicted cluster labels to the true class labels (if provided). This might not work in cases where *num_clust* is large. Please use *sklearn.metrics* for computing metrics in such cases, and provide the correctly matched labels.

See also

sklearn.metrics: Scikit-learn metrics functionality support a wide range of metrics.

3.1.3.2 PKBD

class QuadratiK.spherical_clustering.PKBD

Class for estimating density and generating samples of Poisson-kernel based distribution (PKBD).

Methods

PKBD. dpkb(x, mu, rho[, logdens])	Function for estimating the density function of the PKB distribution.
<pre>PKBD.rpkb(n, mu, rho[, method, random_state])</pre>	Function for generating a random sample from PKBD.

PKBD.**dpkb**(x, mu, rho, logdens=False)

Function for estimating the density function of the PKB distribution.

Parameters

x [numpy.ndarray, pandas.DataFrame] A matrix with a number of columns >= 2.

mu

[float] Location parameter with the same length as the rows of x. Normalized to length one.

rho

[float] Concentration parameter. $\rho \in (0, 1]$.

logdens

[bool, optional] If True, densities d are given as $\log(d)$. Defaults to False.

Returns

density

[numpy.ndarray] An array with the evaluated density values.

PKBD.**rpkb**(*n*, *mu*, *rho*, *method='rejvmf'*, *random_state=None*)

Function for generating a random sample from PKBD. The number of observation generated is determined by n.

Parameters

n [int] Sample size.

mu

[float] Location parameter with the same length as the quantiles.

rho

[float] Concentration parameter. $\rho \in (0, 1]$.

method

[str, optional] String that indicates the method used for sampling observations. The available methods are :

• 'rejvmf': acceptance-rejection algorithm using von Mises-Fisher envelops. (Algorithm in Table 2 of Golzy and Markatou 2020);

• 'rejacg': using angular central Gaussian envelops.
(Algorithm in Table 1 of Sablica et al. 2023);

Defaults to 'rejvmf'.

random state

[int, None, optional.] Seed for random number generation. Defaults to None

Returns

samples

[numpy.ndarray] Generated observations from a poisson kernel-based density. This function returns a list with the matrix of generated observations, the number of tries and the number of acceptance.

References

Golzy M. & Markatou M. (2020) Poisson Kernel-Based Clustering on the Sphere: Convergence Properties, Identifiability, and a Method of Sampling, Journal of Computational and Graphical Statistics, 29:4, 758-770, DOI: 10.1080/10618600.2020.1740713.

Sablica L., Hornik K., Leydold J. "Efficient sampling from the PKBD distribution," Electronic Journal of Statistics, 17(2), 2180-2209, (2023)

Examples

```
>>> from QuadratiK.spherical_clustering import PKBD
>>> pkbd_data = PKBD().rpkb(10,[0.5,0],0.5, "rejvmf", random_state= 42)
>>> dens_val = PKBD().dpkb(pkbd_data, [0.5,0.5],0.5)
>>> print(dens_val)
... [0.46827108 0.05479605 0.21163936 0.06195099 0.39567698 0.40473724
... 0.26561508 0.36791766 0.09324676 0.46847274]
```

3.1.4 User Interface

UI() The UI class is a user interface class that runs a Streamlit dashboard using asyncio.

3.1.4.1 UI

class QuadratiK.ui.UI

The UI class is a user interface class that runs a Streamlit dashboard using asyncio.

Examples

```
>>> from QuadratiK.ui import UI
>>> UI().run()
```

Methods

UI.main()	The <i>main</i> function runs a Streamlit dashboard by executing a command-line command.
UI.run()	The function runs the main function asynchronously using the asyncio library in Python.

async UI.main()

The main function runs a Streamlit dashboard by executing a command-line command.

UI.run()

The function runs the main function asynchronously using the asyncio library in Python.

3.1.5 Datasets

load_wireless_data([desc, return_X_y,]) The wire	eless data frame has 2000 rows and 8 columns.
--	---

3.1.5.1 load wireless data

QuadratiK.datasets.load_wireless_data(desc=False, $return_X_y=False$, $as_dataframe=True$, scaled=False)

The wireless data frame has 2000 rows and 8 columns. The first 7 variables report the measurements of the Wi-Fi signal strength received from 7 Wi-Fi routers in an office location in Pittsburgh (USA). The last column indicates the class labels.

The function load_wireless_data loads a wireless localization dataset.

Read more in the *User Guide*.

Parameters

desc

[boolean, optional] If set to *True*, the function will return the description along with the data. If set to *False*, the description will not be included. Defaults to False.

$return_X_y$

[boolean, optional] Determines whether the function should return the data as separate arrays (*X* and *y*). Defaults to False.

as_dataframe

[boolean, optional] Determines whether the function should return the data as a pandas DataFrame (Trues) or as a numpy array (False). Defaults to True.

scaled

[boolean, optional] Determines whether or not the data should be scaled. If set to True, the data will be divided by its Euclidean norm along each row. Defaults to False.

Returns

(data, target)

[tuple, if return_X_y is True] A tuple of two ndarray. The first containing a 2D array of shape (n_samples, n_features) with each row representing one sample and each column representing the features. The second ndarray of shape (n_samples,) containing the target samples.

data

[pandas.DataFrame, if as_dataframe is True] Dataframe of the data with shape (n_samples, n features + class)

(desc, data, target)

[tuple, if desc is True and return_X_y is True] A tuple of description and two numpy.ndarray. The first containing a 2D array of shape (n_samples, n_features) with each row representing one sample and each column representing the features. The second ndarray of shape (n_samples,) containing the target samples.

(desc, data)

[tuple, if desc is True and as_dataframe is True] A tuple of description and pandas.DataFrame. Dataframe of the data with shape (n_samples, n_features + class)

References

Rohra, J.G., Perumal, B., Narayanan, S.J., Thakur, P., Bhatt, R.B. (2017). User Localization in an Indoor Environment Using Fuzzy Hybrid of Particle Swarm Optimization & Gravitational Search Algorithm with Neural Networks. In: Deep, K., et al. Proceedings of Sixth International Conference on Soft Computing for Problem Solving. Advances in Intelligent Systems and Computing, vol 546. Springer, Singapore. https://doi.org/10.1007/978-981-10-3322-3_27

Source

Bhatt,Rajen. (2017). Wireless Indoor Localization. UCI Machine Learning Repository. https://doi.org/10.24432/C51880.

Examples

```
>>> from QuadratiK.datasets import load_wireless_data
>>> X, y = load_wireless_data(return_X_y=True)
```

3.1.6 Tools

<pre>sample_hypersphere([npoints, ndim, random_state])</pre>	Generate random samples from the hypersphere
stats(x[, y])	The stats function calculates statistics for one or multiple groups of data.
$qq_plot(x[, y, dist])$	The function qq_plot is used to create a quantile-quantile plot, either for a single sample or for two samples.
sphere3d(x[, y])	The function sphere3d creates a 3D scatter plot with a sphere as the surface and data points plotted on it.
plot_clusters_2d(x[, y])	This function plots a 2D scatter plot of data points, with an optional argument to color the points based on a cluster label, and also plots a unit circle.

3.1.6.1 sample_hypersphere

QuadratiK.tools.sample_hypersphere(npoints=100, ndim=3, random_state=None)
Generate random samples from the hypersphere

Parameters

```
npoints
    [int, optional.] The number of points to generate. Default is 100.

ndim
    [int, optional.] The dimensionality of the hypersphere. Default is 3.

random_state
    [int, None, optional.] Seed for random number generation. Defaults to None
```

Returns

data on sphere

[numpy.ndarray] An array containing random vectors sampled uniformly from the surface of the hypersphere.

Examples

```
>>> from QuadratiK.tools import sample_hypersphere
>>> sample_hypersphere(100,3,random_state = 42)
... array([[ 0.60000205, -0.1670153 , 0.78237039],
... [ 0.97717133, -0.15023209, -0.15022156], ......
```

3.1.6.2 stats

```
QuadratiK.tools.stats(x, y=None)
```

The stats function calculates statistics for one or multiple groups of data.

Parameters

y

x [numpy.ndarray, pandas.DataFrame] Data for which statistics is to be calculated.

[numpy.ndarray, pandas.DataFrame, optional] The parameter y is an optional input that can be either another set of observations, or the associated labels for observations (data points).

Returns

summary statistics

[pandas.DataFrame] Summary statistics of the input data.

Examples

```
>>> import numpy as np
>>> from QuadratiK.tools import stats
>>> np.random.seed(42)
>>> X = np.random.randn(100,4)
>>> stats(X)
             Feature 0 Feature 1 Feature 2 Feature 3
   Mean
            -0.009811 0.033746 0.022496
                                             0.043764
   Std Dev 0.868065 0.952234 1.044014
                                             0.982240
   Median
            -0.000248 \quad -0.024646 \quad 0.068665
                                              0.075219
   IQR
             1.244319
                       1.111478 1.318245
                                              1.506492
   Min
            -2.025143 -1.959670 -3.241267
                                             -1.987569
                        3.852731 2.189803
   Max
             2.314659
                                              2.720169
```

3.1.6.3 qq plot

```
QuadratiK.tools.qq_plot(x, y=None, dist='norm')
```

The function qq_plot is used to create a quantile-quantile plot, either for a single sample or for two samples.

Parameters

x [numpy.ndarray] The x parameter represents the data for which you want to create a QQ plot. It can be a single variable or an array-like object containing multiple variables

y [numpy.ndarray, optional] The parameter y is an optional argument that represents the second sample for a two-sample QQ plot. If provided, the function will generate a QQ plot comparing the two samples

dist

[str, optional] Supports all the scipy.stats.distributions. The *dist* parameter specifies the distribution to compare the data against in the QQ plot. By default, it is set to "norm" which represents the normal distribution. However, you can specify a different distribution if you want to compare the data against a different distribution. Defaults to "norm".

Returns

Returns QQ plots.

Examples

```
>>> import numpy as np
>>> from QuadratiK.tools import qq_plot
>>> np.random.seed(42)
>>> X = np.random.randn(100,4)
>>> qq_plot(X)
```

3.1.6.4 sphere3d

```
QuadratiK.tools.sphere3d(x, y=None)
```

The function sphere3d creates a 3D scatter plot with a sphere as the surface and data points plotted on it.

Parameters

[numpy.ndarray, pandas.DataFrame] The parameter x represents the input data for the scatter plot. It should be a 2D array-like object with shape (n_samples, 3), where each row represents the coordinates of a point in 3D space

y [numpy.ndarray, list, optional] The parameter *y* is an optional input that determines the color and shape of each data point in the plot. If *y* is not provided, the scatter plot will have the default marker symbol and color.

Returns

Returns a 3D plot of a sphere with data points plotted on it.

Examples

```
>>> from QuadratiK.tools import sphere3d
>>> np.random.seed(42)
>>> X = np.random.randn(100,3)
>>> sphere3d(X)
```

3.1.6.5 plot_clusters_2d

```
QuadratiK.tools.plot_clusters_2d(x, y=None)
```

This function plots a 2D scatter plot of data points, with an optional argument to color the points based on a cluster label, and also plots a unit circle.

Parameters

x [numpy.ndarray, pandas.DataFrame] The parameter x is a 2-dimensional array or matrix containing the coordinates of the data points to be plotted. Each row of x represents the coordinates of a single data point in the 2-dimensional space

y [numpy.ndarray, pandas.DataFrame, optional] The parameter *y* is an optional array that represents the labels or cluster assignments for each data point in *x*. If *y* is provided, the data points will be colored according to their labels or cluster assignments.

Returns

A matplotlib figure object.

Examples

```
>>> import numpy as np
>>> from QuadratiK.tools import plot_clusters_2d
>>> np.random.seed(42)
>>> X = np.random.randn(100,2)
>>> X = X/np.linalg.norm(X,axis = 1, keepdims=True)
>>> plot_clusters_2d(X)
```

CHAPTER

FOUR

USER GUIDE

4.1 User Guide

4.1.1 Dataset

4.1.1.1 Wireless Indoor Localization Dataset

The *wireless* data frame has 2000 rows and 8 columns. The first 7 variables report the measurements of the Wi-Fi signal strength received from 7 Wi-Fi routers in an office location in Pittsburgh (USA). The last column indicates the class labels.

Format

A data frame containing the following columns:

- V1: signal strength from router 1.
- V2: signal strength from router 2.
- *V3*: signal strength from router 3.
- V4: signal strength from router 4.
- V5: signal strength from router 5.
- V6: signal strength from router 6.
- *V7*: signal strength from router 7.
- V8: group memberships, from 1 to 4.

Details

The Wi-Fi signal strength is measured in dBm, decibel milliwatts, which is expressed as a negative value ranging from -100 to 0. The labels correspond to 'conference room', 'kitchen', 'indoor sports room', and 'other'. In total, we have 4 groups with 500 observations each.

Source

Bhatt, Rajen. (2017). Wireless Indoor Localization. UCI Machine Learning Repository. https://doi.org/10.24432/

References

Rohra, J.G., Perumal, B., Narayanan, S.J., Thakur, P., Bhatt, R.B. (2017). User Localization in an Indoor Environment Using Fuzzy Hybrid of Particle Swarm Optimization & Gravitational Search Algorithm with Neural Networks. In: Deep, K., et al. Proceedings of Sixth International Conference on Soft Computing for Problem Solving. Advances in Intelligent Systems and Computing, vol 546. Springer, Singapore. https://doi.org/10.1007/978-981-10-3322-3_27

4.1.2 Usage Examples

4.1.2.1 QuadratiK Usage Examples

Normality Test

This section contains example for the Parametric and Non-parametric Normality Test based on kernel-based quadratic distances

Parametric

```
[1]: import numpy as np
    from QuadratiK.kernel_test import KernelTest
    np.random.seed(42)
    data = np.random.randn(100,2)
    normality_test = KernelTest(h=0.4, centering_type="param",random_state=42).test(data)
    print("Test : {}".format(normality_test.test_type_))
    print("Execution time: {:.3f}".format(normality_test.execution_time))
    print("H0 is Rejected : {}".format(normality_test.h0_rejected_))
    print("Test Statistic : {}".format(normality_test.test_statistic_))
    print("Critical Value (CV) : {}".format(normality_test.cv_))
    print("CV Method : {}".format(normality_test.cv_method_))
    print("Selected tuning parameter : {}".format(normality_test.h))
    Test: Kernel-based quadratic distance Normality test
    Execution time: 1.578
    HO is Rejected : False
    Test Statistic: -0.004422397826208057
    Critical Value (CV): 0.00495159345113745
    CV Method : Empirical
    Selected tuning parameter: 0.4
```

```
[2]: print(normality_test.summary())
    Time taken for execution: 1.578 seconds
    Test Results
```

4.1. User Guide 27

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Test Type Test Stati Critical V	istic -0.004	-based quadrati 422397826208057 5159345113745	ic distance Normality test 7
Reject H0		3139343113743	
Summary St	 -atistics		
Summary St		Feature 1	
	0 11FC	0.024	
Mean Std Dev	-0.1156 0.8563	0.034 0.9989	
Median	-0.0353	0.1323	
IQR	1.0704	1.3333	
Min	-2.6197	-1.9876	
Max	1.8862	2.7202	

Non-parametric

```
[3]: normality_test = KernelTest(h=0.4, centering_type="nonparam").test(data)
    print("Test : {}".format(normality_test.test_type_))
    print("Execution time: {:.3f}".format(normality_test.execution_time))
    print("H0 is Rejected : {}".format(normality_test.h0_rejected_))
    print("Test Statistic : {}".format(normality_test.test_statistic_))
    print("Critical Value (CV) : {}".format(normality_test.cv_))
    print("CV Method : {}".format(normality_test.cv_method_))
    print("Selected tuning parameter : {}".format(normality_test.h))

Test : Kernel-based quadratic distance Normality test
    Execution time: 0.131
    H0 is Rejected : False
    Test Statistic : 0.0015387891795935942
    Critical Value (CV) : 0.0020181255711485594
    CV Method : Empirical
    Selected tuning parameter : 0.4
```

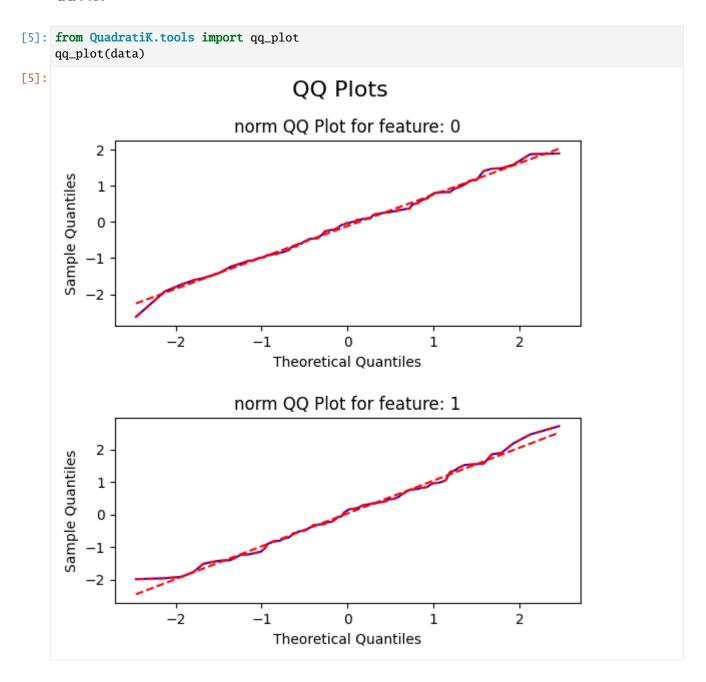
[4]: print(normality_test.summary())

```
Time taken for execution: 0.131 seconds
Test Results
_____
Test Type Kernel-based quadratic distance Normality test
Test Statistic 0.0015387891795935942
Critical Value 0.0020181255711485594
Reject H0
            False
_____
Summary Statistics
       Feature 0 Feature 1
Mean
         -0.1156
                     0.034
                     0.9989
Std Dev
         0.8563
Median
         -0.0353
                     0.1323
IOR
          1.0704
                     1.3333
```

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QQ Plot



Two Sample Test

This sections shows example for the two-sample test using normal kernel-based quadratic distance

```
[6]: import numpy as np
    from QuadratiK.kernel_test import KernelTest
    np.random.seed(42)
    X = np.random.randn(100,2)
    np.random.seed(42)
    Y = np.random.randn(100,2)
    two_sample_test = KernelTest(h=0.4, random_state=42).test(X,Y)
    print("Test : {}".format(two_sample_test.test_type_))
    print("Execution time: {:.3f}".format(two_sample_test.execution_time))
    print("H0 is Rejected : {}".format(two_sample_test.h0_rejected_))
    print("Test Statistic : {}".format(two_sample_test.test_statistic_))
    print("Critical Value (CV) : {}".format(two_sample_test.cv_))
    print("CV Method : {}".format(two_sample_test.cv_method_))
    print("Selected tuning parameter : {}".format(two_sample_test.h))
    Test : Kernel-based quadratic distance two-sample test
    Execution time: 0.041
    HO is Rejected: False
    Test Statistic: -0.018355578706893333
    Critical Value (CV): 0.011282236253872464
    CV Method: subsampling
    Selected tuning parameter: 0.4
[7]: print(two_sample_test.summary())
    Time taken for execution: 0.041 seconds
    Test Results
              Kernel-based quadratic distance two-sample test
    Test Type
    Test Statistic -0.018355578706893333
    Critical Value 0.011282236253872464
    Reject H0
                   False
    Summary Statistics
                               Group 1 Group 2
                                                    Overall
                             _____
    ('Feature 0', 'Mean')
                               -0.1156 -0.1156 -0.1156
    ('Feature 0', 'Std Dev')
                               0.8563 0.8563
                                                    0.8542
    ('Feature 0', 'Median')
                               -0.0353
                                          -0.0353
                                                     -0.0353
    ('Feature 0', 'IQR')
                               1.0704
                                          1.0704
                                                    1.0704
    ('Feature 0', 'Min')
                               -2.6197
                                          -2.6197
                                                    -2.6197
    ('Feature 0', 'Max')
                                1.8862
                                           1.8862
                                                     1.8862
    ('Feature 1', 'Mean')
                                0.034
                                           0.034
                                                     0.034
    ('Feature 1', 'Std Dev')
                                0.9989
                                           0.9989
                                                     0.9963
    ('Feature 1', 'Median')
                                0.1323
                                           0.1323
                                                     0.1323
    ('Feature 1', 'IQR')
                                1.3333
                                          1.3333
                                                     1.3333
    ('Feature 1', 'Min')
                               -1.9876
                                          -1.9876
                                                     -1.9876
    ('Feature 1', 'Max')
                                2.7202
                                           2.7202
                                                     2.7202
```

K-Sample Test

→0789

('Feature 1', 'Mean')

Shows examples for the kernel-based quadratic distance k-sample tests with the Normal kernel and bandwidth parameter h.

```
[8]: from QuadratiK.kernel_test import KernelTest
    np.random.seed(42)
    X = np.random.randn(500,2)
    np.random.seed(42)
    y = np.random.randint(0,5,500)
    k_sample_test = KernelTest(h = 1.5, method = "permutation").test(X,y)
    print("Test : {}".format(k_sample_test.test_type_))
    print("Execution time: {:.3f} seconds".format(k_sample_test.execution_time))
    print("H0 is Rejected : {}".format(k_sample_test.h0_rejected_))
    print("Test Statistic : {}".format(k_sample_test.test_statistic_))
    print("Critical Value (CV) : {}".format(k_sample_test.cv_))
    print("CV Method : {}".format(k_sample_test.cv_method_))
    print("Selected tuning parameter : {}".format(k_sample_test.h))
    Test : Kernel-based quadratic distance K-sample test
    Execution time: 0.248 seconds
    HO is Rejected : False
    Test Statistic : [0.00140789 0.00035197]
    Critical Value (CV) : [0.00431479 0.0010787 ]
    CV Method : permutation
    Selected tuning parameter: 1.5
[9]: print(k_sample_test.summary())
    Time taken for execution: 0.248 seconds
    Test Results
    Test Type Kernel-based quadratic distance K-sample test
    Test Statistic [0.00140789 0.00035197]
    Critical Value [0.00431479 0.0010787 ]
                False
    Reject H0
    Summary Statistics
                               Group 0
                                          Group 1 Group 2
                                                               Group 3
                                                                          Group 4
     ⊶0verall
    ('Feature 0', 'Mean') 0.033 -0.1227
                                                     0.0547
                                                               -0.0554 0.1192
                                                                                      0.
     →0036
    ('Feature 0', 'Std Dev') 1.0563
('Feature 0', 'Median') 0.0485
                                          0.874
                                                      0.8279
                                                                0.9351
                                                                           1.1038
                                                                                      0.967
    ('Feature 0', 'Median')
                                0.0485
                                          -0.0347
                                                      0.0675
                                                               -0.0349
                                                                           0.1958
                                                                                      0.
     →0184
    ('Feature 0', 'IQR')
                                                                                     1.239
                               1.4214
                                           1.0371
                                                     0.9924
                                                               1.1388
                                                                          1.3338
    ('Feature 0', 'Min')
                                                                                     -3.
                               -2.6969
                                          -2.0819
                                                    -1.7787
                                                               -2.651
                                                                         -3.2413
     →2413
    ('Feature 0', 'Max')
                                           2.2989
                                                    2.1898
                                                               2.4458
                                                                           3.0789
                                                                                      3.
                               2.5269
```

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0.1786

4.1. User Guide 31

-0.0934

-0.0257

0.072

0.0501

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	1.0116	1.0488	0.9651	0.9411	0.9945	0.992
('Feature 1', 'Median') ⇔0283	0.0481	0.1714	-0.1857	-0.1872	0.2239	0.
('Feature 1', 'IQR') ⇒3616	1.2537	1.3063	1.2909	1.3971	1.4369	1.
('Feature 1', 'Min') 4239	-2.0417	-2.3019	-2.0392	-2.4239	-2.2111	-2.
('Feature 1', 'Max') →8527	3.8527	2.6324	2.7202	2.4632	2.1905	3.

Poisson Kernel Test

Shows example for perforing the the kernel-based quadratic distance Goodness-of-fit tests for Uniformity for spherical data using the Poisson kernel with concentration parameter rho.

```
[10]: from QuadratiK.tools import sample_hypersphere
     from QuadratiK.poisson_kernel_test import PoissonKernelTest
     np.random.seed(42)
     X = sample_hypersphere(100,3, random_state=42)
     unif_test = PoissonKernelTest(rho = 0.7, random_state=42).test(X)
     print("Execution time: {:.3f} seconds".format(unif_test.execution_time))
     print("U Statistic Results")
     print("H0 is rejected : {}".format(unif_test.u_statistic_h0_))
     print("Un Statistic : {}".format(unif_test.u_statistic_un_))
     print("Critical Value : {}".format(unif_test.u_statistic_cv_))
     print("V Statistic Results")
     print("H0 is rejected : {}".format(unif_test.v_statistic_h0_))
     print("Vn Statistic : {}".format(unif_test.v_statistic_vn_))
     print("Critical Value : {}".format(unif_test.v_statistic_cv_))
     Execution time: 0.041 seconds
     U Statistic Results
     HO is rejected: False
     Un Statistic: 1.6156682048968174
     Critical Value: 0.06155875299050079
     V Statistic Results
     HO is rejected: False
     Vn Statistic: 22.83255917641962
     Critical Value: 23.229486935225513
```

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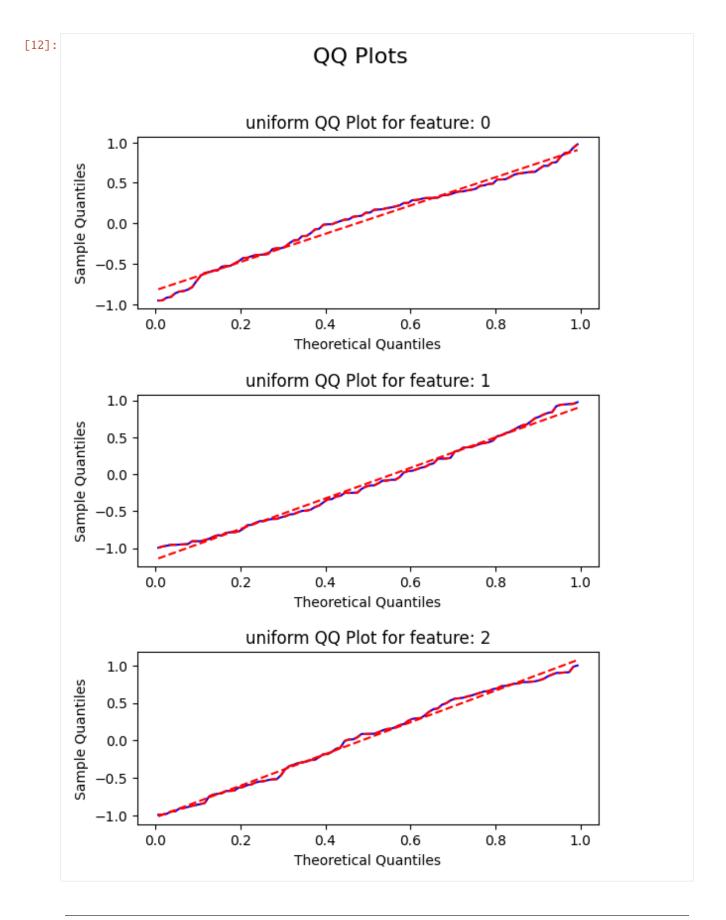
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U Statist	tic Un	1.61566	82048968174
U Statistic Reject HO		alue 0.06155	875299050079
		False	
		22.8325	22.83255917641962
V Statist	tic Critical V	alue 23.2294	86935225513
V Statist	tic Reject H0	False	
Summary S	Statistics		
	Feature 0	Feature 1	Feature 2
Mean	0.0451	-0.1206	0.0309
Std Dev	0.509		
Median	0.132	-0.1596	0.0879
IQR	0.8051	1.0063	1.1473
Min	-0.9548	-0.9929	-0.9904
Max	0.9772	0.9738	0.9996

QQ Plot

```
[12]: from QuadratiK.tools import qq_plot

qq_plot(X,dist = "uniform")
```



Poisson Kernel based Clustering

Shows example for performing the Poisson kernel-based clustering algorithm on the Sphere based on the Poisson kernel-based densities.

```
[13]: from QuadratiK.datasets import load_wireless_data
     from QuadratiK.spherical_clustering import PKBC
     from sklearn.preprocessing import LabelEncoder
     X, y = load_wireless_data(return_X_y=True)
     le = LabelEncoder()
     le.fit(v)
     y = le.transform(y)
     cluster_fit = PKBC(num_clust=4, random_state=42).fit(X)
     ari, macro_precision, macro_recall, avg_silhouette_Score = cluster_fit.validation(y)
     print("Estimated mixing proportions :", cluster_fit.alpha_)
     print("Estimated concentration parameters: ", cluster_fit.rho_)
     print("Adjusted Rand Index:", ari)
     print("Macro Precision:", macro_precision)
     print("Macro Recall:", macro_recall)
     print("Average Silhouette Score:", avg_silhouette_Score)
     Estimated mixing proportions: [0.23590339 0.24977919 0.25777522 0.25654219]
     Estimated concentration parameters: [0.97773265 0.98348976 0.98226901 0.98572597]
     Adjusted Rand Index: 0.9403086353805835
     Macro Precision: 0.9771870612442508
     Average Silhouette Score: 0.3803089203572107
```

Elbow Plot using Euclidean Distance and Cosine Similarity based WCSS

```
[14]: import matplotlib.pyplot as plt

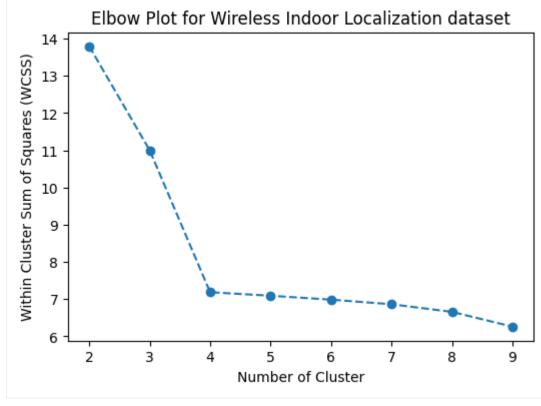
wcss_euc = []
wcss_cos = []

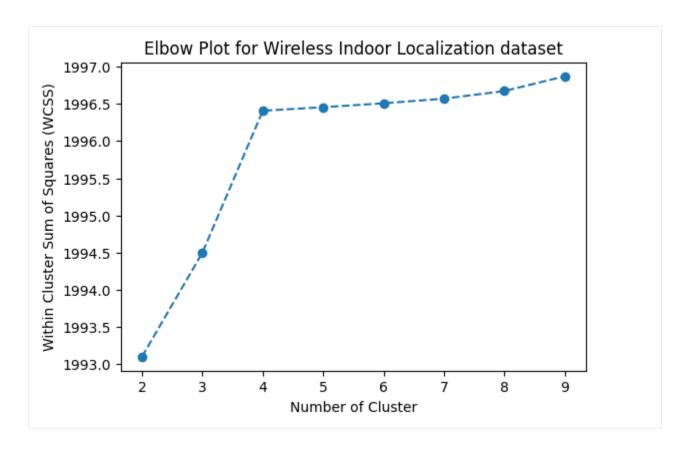
for i in range(2, 10):
    clus_fit = PKBC(num_clust=i).fit(X)
    wcss_euc.append(clus_fit.euclidean_wcss_)
    wcss_cos.append(clus_fit.cosine_wcss_)

fig = plt.figure(figsize=(6, 4))
plt.plot(list(range(2, 10)), wcss_euc, "--o")
plt.xlabel("Number of Cluster")
plt.ylabel("Within Cluster Sum of Squares (WCSS)")
plt.title("Elbow Plot for Wireless Indoor Localization dataset")
plt.show()
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```

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```
fig = plt.figure(figsize=(6, 4))
plt.plot(list(range(2,10)),wcss_cos, "--o")
plt.xlabel("Number of Cluster")
plt.ylabel("Within Cluster Sum of Squares (WCSS)")
plt.title("Elbow Plot for Wireless Indoor Localization dataset")
plt.show()
```





Density Estimation and Sample Generation from PKBD

```
[15]: from QuadratiK.spherical_clustering import PKBD
pkbd_data = PKBD().rpkb(10,[0.5,0],0.5, "rejvmf", random_state= 42)
dens_val = PKBD().dpkb(pkbd_data, [0.5,0.5],0.5)
print(dens_val)

[0.46827108 0.05479605 0.21163936 0.06195099 0.39567698 0.40473724
0.26561508 0.36791766 0.09324676 0.46847274]
```

Tuning Parameter *h* **selection**

Computes the kernel bandwidth of the Gaussian kernel for the two-sample and ksample kernel-based quadratic distance (KBQD) tests.

```
[16]: import numpy as np
    from QuadratiK.kernel_test import select_h
    np.random.seed(42)
    X = np.random.randn(200, 2)
    np.random.seed(42)
    y = np.random.randint(0, 2, 200)
    h_selected, all_values, power_plot = select_h(
         X, y, alternative='location', power_plot=True, random_state=None)
    print("Selected h is: ", h_selected)
```

Selected h is: 2.8

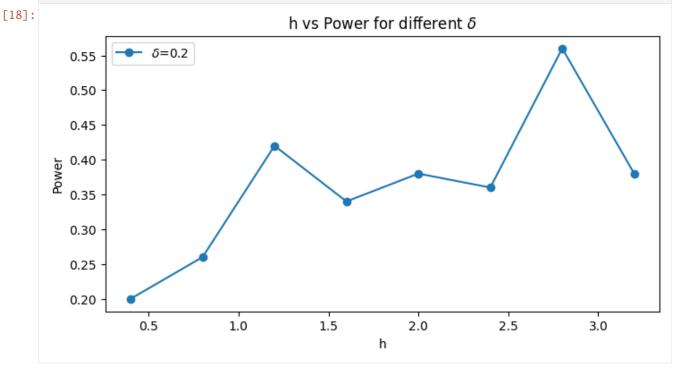
[17]: #shows the detailed power vs h table all_values [17]: h delta power 0 0.4 0.2 0.20 0.2 0.26 1 0.8 1.2 0.2 0.42 1.6 0.2 0.34 4 2.0 0.2 0.38 5 2.4 0.2 0.36 6 2.8 0.2 0.56

[18]: #shows the power plot power_plot

0.2

0.38

7 3.2



PYTHON MODULE INDEX

q

QuadratiK.datasets, 20 QuadratiK.kernel_test, 5 QuadratiK.poisson_kernel_test, 11 QuadratiK.spherical_clustering, 14 QuadratiK.tools, 22 QuadratiK.ui, 19

INDEX

D dpkb() (QuadratiK.spherical_clustering.PKBD method), 18	<pre>module, 13 QuadratiK.tools module, 21 QuadratiK.ui module, 19</pre>
fit() (QuadratiK.spherical_clustering.PKBC method), 16 K KernelTest (class in QuadratiK.kernel_test), 5	R rpkb() (QuadratiK.spherical_clustering.PKBD method), 18 run() (QuadratiK.ui.UI method), 20 S
L load_wireless_data() (in module	sample_hypersphere() (in module QuadratiK.tools), 22 select_h() (in module QuadratiK.kernel_test), 9 sphere3d() (in module QuadratiK.tools), 24 stats() (in module QuadratiK.tools), 23 stats() (QuadratiK.kernel_test.KernelTest method), 8 stats() (QuadratiK.poisson_kernel_test.PoissonKernelTest method), 13 stats() (QuadratiK.spherical_clustering.PKBC method), 16 summary() (QuadratiK.kernel_test.KernelTest method), 8 summary() (QuadratiK.poisson_kernel_test.PoissonKernelTest method), 13
PKBC (class in QuadratiK.spherical_clustering), 14 PKBD (class in QuadratiK.spherical_clustering), 17 plot_clusters_2d() (in module QuadratiK.tools), 25 PoissonKernelTest (class in QuadratiK.poisson_kernel_test), 11	T test() (QuadratiK.kernel_test.KernelTest method), 8 test() (QuadratiK.poisson_kernel_test.PoissonKernelTest
Q	U UI (class in QuadratiK.ui), 19
<pre>qq_plot() (in module QuadratiK.tools), 23 QuadratiK.datasets module, 20 QuadratiK.kernel_test module, 5 QuadratiK.poisson_kernel_test module, 11 QuadratiK.spherical_clustering</pre>	V validation() (QuadratiK.spherical_clustering.PKBC method), 16