Tutorial on the R package TDA

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Abstract

This tutorial gives an introduction to the R package **TDA**, which provides some tools for Topological Data Analysis. The salient topological features of data can be quantified with persistent homology. The R package **TDA** provide an R interface for the efficient algorithms of the C++ libraries **GUDHI**, **Dionysus**, and **PHAT**. Specifically, The R package **TDA** includes functions for computing the persistent homology of the Rips complex, alpha complex, and alpha shape complex, and a function for the persistent homology of sublevel sets (or superlevel sets) of arbitrary functions evaluated over a grid of points. The R package **TDA** also provides a function for computing the confidence band that determines the significance of the features in the resulting persistence diagrams.

Keywords: Topological Data Analysis, Persistent Homology.

1. Introduction

R(http://cran.r-project.org/) is a programming language for statistical computing and graphics.

R has several good properties: R has many packages for statistical computing. Also, R is easy to make (interactive) plots. R is a script language, and it is easy to use. But, R is slow. C or C++ stands on the opposite end: C or C++ also has many packages(or libraries). But, C or C++ is difficult to make plots. C or C++ is a compiler language, and is difficult to use. But, C or C++ is fast. In short, R has short development time but long execution time, and C or C++ has long development time but short execution time.

Several libraries are developed for Topological Data Analysis: for example, **GUDHI**(https://project.inria.fr/gudhi/software/), **Dionysus**(http://www.mrzv.org/software/dionysus/), and **PHAT**(https://code.google.com/p/phat/). They are all written in C++, since Topological Data Analysis is computationally heavy and R is not fast enough.

R package **TDA**(http://cran.r-project.org/web/packages/TDA/index.html) bridges between C++ libraries(**GUDHI**, **Dionysus**, **PHAT**) and R. **TDA** package provides an R interface for the efficient algorithms of the C++ libraries **GUDHI**, **Dionysus** and **PHAT**. So by using **TDA** package, short development time and short execution time can be both achieved.

R package **TDA** provides tools for Topological Data Analysis. You can compute several different things with **TDA** package: you can compute common distance functions and density estimators, the persistent homology of the Rips filtration, the persistent homology of sublevel sets of a function over a grid, the confidence band for the persistence diagram, and the cluster density trees for density clustering.

2. Installation

First, you should download R. R of version at least 3.1.0 is required:

http://cran.r-project.org/bin/windows/base/ (for Windows)

http://cran.r-project.org/bin/macosx/ (for (Mac) OS X)

R is part of many Linux distributions, so you should check with your Linux package management system.

You can use whatever IDE that you would like to use(Rstudio, Eclipse, Emacs, Vim...). R itself also provides basic GUI or CUI. I personally use Rstudio:

http://www.rstudio.com/products/rstudio/download/

For Windows and Mac, you can install R package **TDA** as in the following code (or pushing 'Install R packages' button if you use Rstudio).

```
###########################################################################
# installing R package TDA
###########################################################################
if (!require(package = "TDA")) {
  install.packages(pkgs = "TDA")
}

## Loading required package:  TDA
## Warning:  package 'TDA' was built under R version 3.4.4
```

If you are using Linux, you should install R package **TDA** from the source. To do this, you need to install two libraries in advance: gmp (https://gmplib.org/) and mpfr (http://www.mpfr.org/). Installation of these packages may differ by your Linux distributions. Once those libraries are installed, you need to install four R packages: **parallel**, **FNN**, **igraph**, and **scales**. **parallel** is included when you install R, so you need to install **FNN**, **igraph**, and **scales** by yourself. You can install them by following code (or pushing 'Install R packages' button if you use Rstudio).

```
###########################################################################
# installing required packages
###########################################################################
if (!require(package = "FNN")) {
  install.packages(pkgs = "FNN")
}

## Loading required package:  FNN

if (!require(package = "igraph")) {
  install.packages(pkgs = "igraph")
}

## Loading required package:  igraph
##
## Attaching package:  'igraph'
## The following object is masked from 'package:FNN':
##
##     knn
## The following objects are masked from 'package:stats':
##
##     decompose, spectrum
## The following object is masked from 'package:base':
##
##     union

if (!require(package = "scales")) {
  install.packages(pkgs = "scales")
}

## Loading required package:  scales
```

Then you can install the R package **TDA** as in Windows or Mac:

```
##########################################################################
# installing R package TDA
##########################################################################
if (!require(package = "TDA")) {
  install.packages(pkgs = "TDA")
}
```

Once installation is done, R package **TDA** should be loaded as in the following code, before using the package functions.

```
##########################################################################
# loading R package TDA
##########################################################################
library(package = "TDA")
```

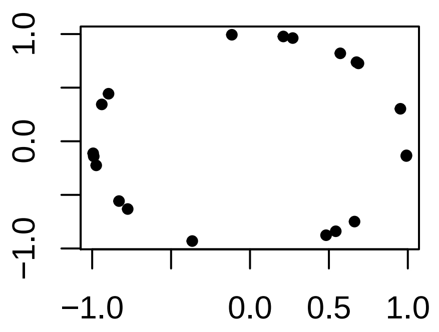
3. Sample on manifolds, Distance Functions, and Density Estimators

3.1. Uniform Sample on manifolds

A set of n points $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ has been sampled from some distribution P.

- n sample from the uniform distribution on the circle in $\mathbb{R}^2$ with radius r.

```
##########################################################################
# uniform sample on the circle
##########################################################################
circleSample <- circleUnif(n = 20, r = 1)
plot(circleSample, xlab = "", ylab = "", pch = 20)
```



3.2. Density Estimators

We compute density estimators over a grid of points. Suppose a set of points $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ has been sampled from some distribution P. The following code generates a sample of 400 points from the unit circle and constructs a grid of points over which we will evaluate the functions.

```
###########################################################################
# uniform sample on the circle, and grid of points
###########################################################################
X <- circleUnif(n = 400, r = 1)

lim <- c(-1.7, 1.7)
by <- 0.05
margin <- seq(from = lim[1], to = lim[2], by = by)
Grid <- expand.grid(margin, margin)
```

- The Gaussian Kernel Density Estimator (KDE), for each $y \in \mathbb{R}^d$, is defined as

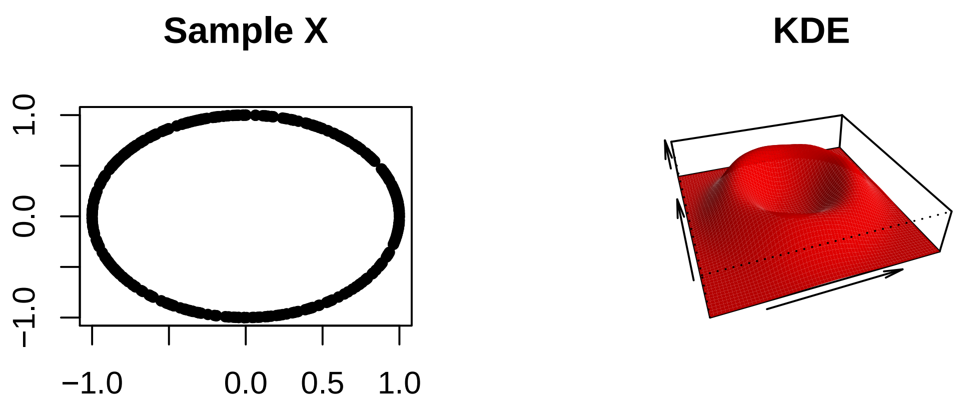
$$\hat{p}_h(y) = \frac{1}{n(\sqrt{2\pi}h)^d} \sum_{i=1}^{n} \exp\left(\frac{-\|y - x_i\|_2^2}{2h^2}\right).$$

  where h is a smoothing parameter.

```
###########################################################################
# kernel density estimator
###########################################################################
h <- 0.3
KDE <- kde(X = X, Grid = Grid, h = h)

par(mfrow = c(1,2))
```

```
plot(X, xlab = "", ylab = "", main = "Sample X", pch = 20)
persp(x = margin, y = margin,
      z = matrix(KDE, nrow = length(margin), ncol = length(margin)),
      xlab = "", ylab = "", zlab = "", theta = -20, phi = 35, scale = FALSE,
      expand = 3, col = "red", border = NA, ltheta = 50, shade = 0.5,
      main = "KDE")
```



4. Persistent Homology

4.1. Persistent Homology Over a Grid

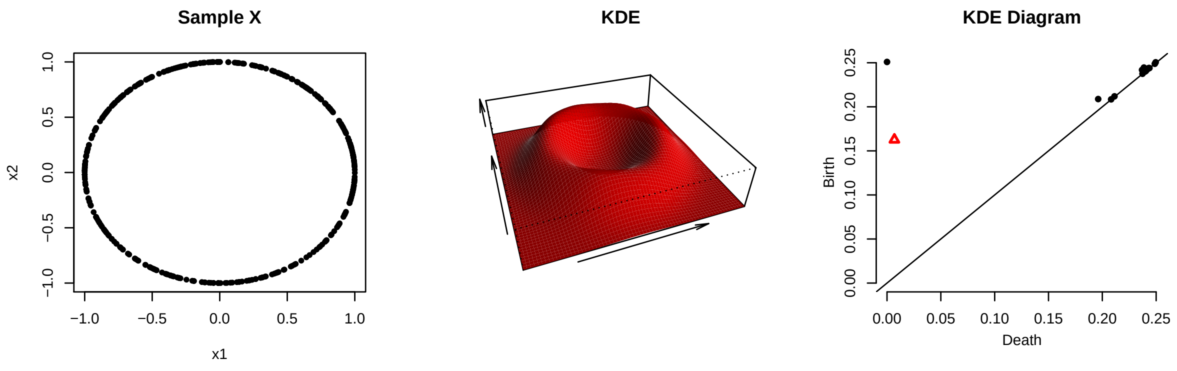
`gridDiag` function computes the persistent homology of sublevel (and superlevel) sets of the functions. The function `gridDiag` evaluates a given real valued function over a triangulated grid (in arbitrary dimension), constructs a filtration of simplices using the values of the function, and computes the persistent homology of the filtration. The user can choose to compute persistence diagrams using either the C++ library **GUDHI** (`library = "GUDHI"`), **Dionysus** (`library = "Dionysus"`), or **PHAT** (`library = "PHAT"`) .

The following code computes the persistent homology of the superlevel sets (`sublevel = FALSE`) of the kernel density estimator (`FUN = kde`, `h = 0.3`) using the point cloud stored in the matrix `X` from the previous example. The other inputs are the features of the grid over which the `kde` is evaluated (`lim` and `by`), and a logical variable that indicates whether a progress bar should be printed (`printProgress`).

```
##########################################################################
# persistent homology of a function over a grid
##########################################################################
DiagGrid <- gridDiag(X = X, FUN = kde, lim = cbind(lim, lim), by = by,
    sublevel = FALSE, library = "Dionysus", printProgress = FALSE, h = 0.3)
```

The function `plot` plots persistence diagram for objects of the class `"diagram"`.

```
#################################################################################
# plotting persistence diagram
#################################################################################
par(mfrow = c(1,3))
plot(X, main = "Sample X", pch = 20)
persp(x = margin, y = margin,
      z = matrix(KDE, nrow = length(margin), ncol = length(margin)),
      xlab = "", ylab = "", zlab = "", theta = -20, phi = 35, scale = FALSE,
      expand = 3, col = "red", border = NA, ltheta = 50, shade = 0.9,
      main = "KDE")
plot(x = DiagGrid[["diagram"]], main = "KDE Diagram")
```



4.2. Rips Persistent Homology

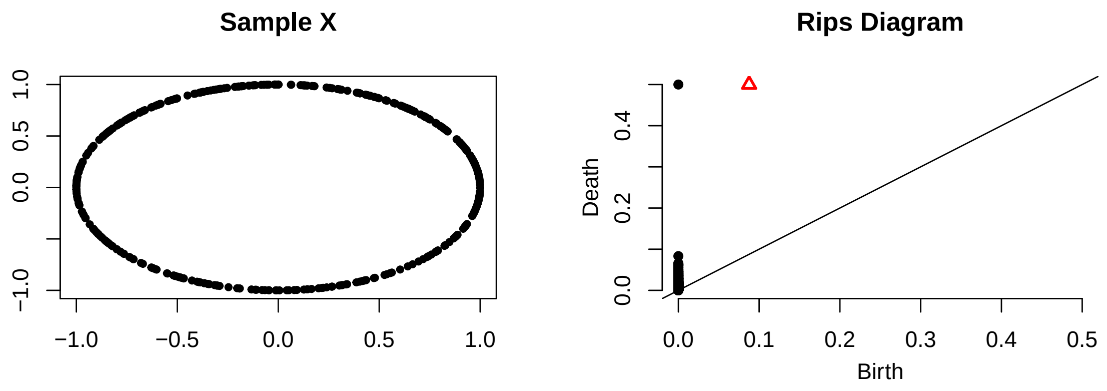
The *Vietoris-Rips complex* $R(X, \varepsilon)$ consists of simplices with vertices in $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ and diameter at most ε. In other words, a simplex σ is included in the complex if each pair of vertices in σ is at most ε apart. The sequence of Rips complexes obtained by gradually increasing the radius ε creates a filtration.

The `ripsDiag` function computes the persistence diagram of the Rips filtration built on top of a point cloud. The user can choose to compute the Rips filtration using either the C++ library **GUDHI** or **Dionysus**. Then for computing the persistence diagram from the Rips filtration, the user can use either the C++ library **GUDHI**, **Dionysus**, or **PHAT**.

The following code computes the persistent homology of the Rips filtratio using the point cloud stored in the matrix `X` from the previous example, and the plot the data and the diagram.

```
DiagRips <- ripsDiag(X = X, maxdimension = 1, maxscale = 0.5,
    library = c("GUDHI", "Dionysus"), location = TRUE)

par(mfrow = c(1,2))
plot(X, xlab = "", ylab = "", main = "Sample X", pch = 20)
plot(x = DiagRips[["diagram"]], main = "Rips Diagram")
```



4.3. Persistent Homology from filtration

Rather than computing persistence diagrams from built-in function, it is also possible to compute persistence diagrams from a user-defined filtration. A filtration consists of simplicial complex and the filtration values on each simplex. The functions `ripsDiag` has their counterparts for computing corresponding filtrations instead of persistence diagrams: namely, `ripsFiltration` corresponds to the Rips filtration built on top of a point cloud.

After specifying the limit of the Rips filtration and the max dimension of the homological features, the following code compute the Rips filtration using the point cloud `X`.

```
FltRips <- ripsFiltration(X = X, maxdimension = 1, maxscale = 0.5,
    library = "GUDHI")
```

One way of defining a user-defined filtration is to build a filtration from a simplicial complex and function values on the vertices. The function `funFiltration` takes function values (`FUNvalues`) and simplicial complex (`cmplx`) as input, and build a filtration, where a filtration value on a simplex is defined as the maximum of function values on the vertices of the simplex.

In the following example, the function `funFiltration` construct a filtration from a Rips complex and the kernel density estimates on data points.

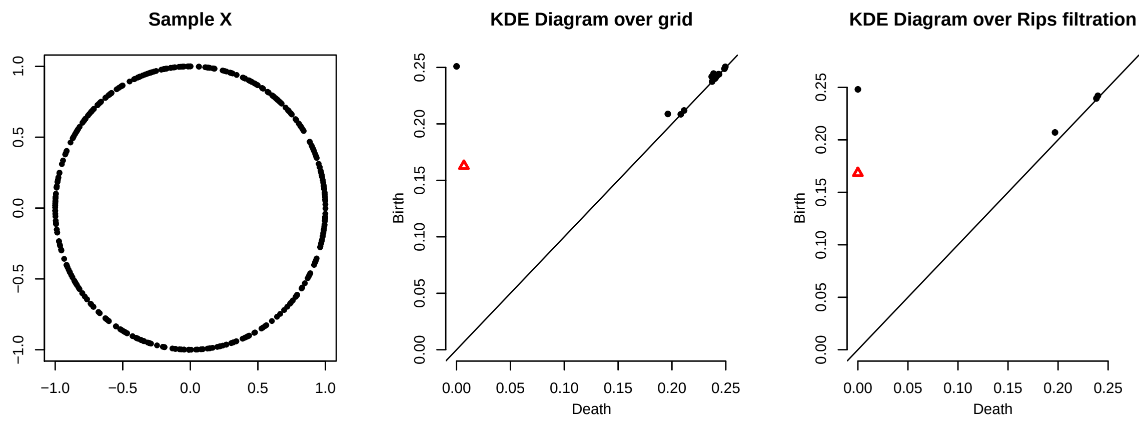
```
h <- 0.3
KDEx <- kde(X = X, Grid = X, h = h)

FltFun <- funFiltration(FUNvalues = KDEx, cmplx = FltRips[["cmplx"]],
    sublevel = FALSE)
```

Once the filtration is computed, the function `filtrationDiag` computes the persistence diagram from the filtration. The user can choose to compute the persistence diagram using either the C++ library **GUDHI** or **Dionysus**.

```
DiagFltFun <- filtrationDiag(filtration = FltFun, maxdimension = 1,
    library = "Dionysus", location = TRUE, printProgress = FALSE)

par(mfrow = c(1,3))
plot(X, xlab = "", ylab = "", main = "Sample X", pch = 20)
plot(x = DiagGrid[["diagram"]], main = "KDE Diagram over grid")
plot(x = DiagFltFun[["diagram"]], diagLim = c(0, 0.27),
    main = "KDE Diagram over Rips filtration")
```



5. Statistical Inference on Persistent Homology

$(1-\alpha)$ confidence band can be computed for a function using the bootstrap algorithm, which we briefly describe using the kernel density estimator:

1. Given a sample $X = \{x_1, \ldots, x_n\}$, compute the kernel density estimator $\hat{p}_h$;
2. Draw $X^* = \{x_1^*, \ldots, x_n^*\}$ from $X = \{x_1, \ldots, x_n\}$ (with replacement), and compute $\theta^* = \sqrt{n}\|\hat{p}_h^*(x) - \hat{p}_h(x)\|_\infty$, where $\hat{p}_h^*$ is the density estimator computed using X^*;
3. Repeat the previous step B times to obtain $\theta_1^*, \ldots, \theta_B^*$;
4. Compute $q_\alpha = \inf\left\{q : \frac{1}{B}\sum_{j=1}^{B} I(\theta_j^* \geq q) \leq \alpha\right\}$;
5. The $(1-\alpha)$ confidence band for $\mathbb{E}[\hat{p}_h]$ is $\left[\hat{p}_h - \frac{q_\alpha}{\sqrt{n}}, \hat{p}_h + \frac{q_\alpha}{\sqrt{n}}\right]$.

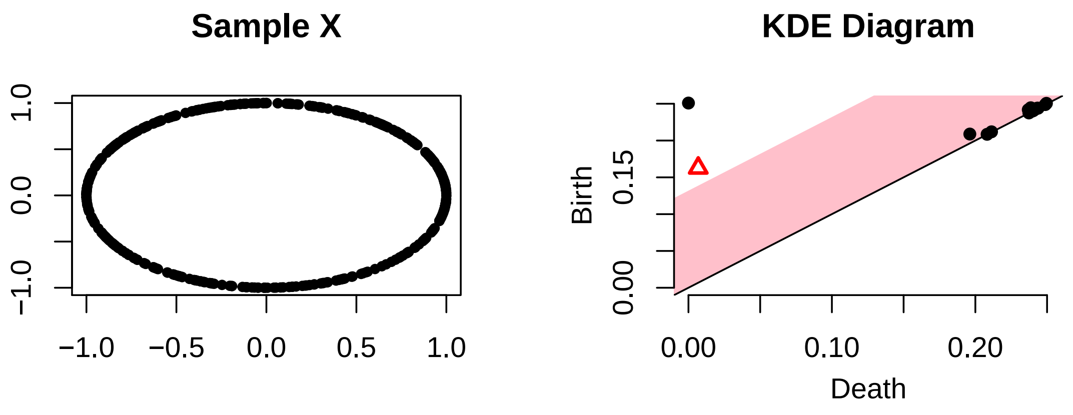
`bootstrapBand` computes $(1-\alpha)$ bootstrap confidence band, with the option of parallelizing the algorithm (`parallel=TRUE`). The following code computes a 90% confidence band for $\mathbb{E}[\hat{p}_h]$.

```
##########################################################################
# bootstrap confidence band for kde function
##########################################################################
bandKDE <- bootstrapBand(X = X, FUN = kde, Grid = Grid, B = 100,
                         parallel = FALSE, alpha = 0.1, h = h)
print(bandKDE[["width"]])

##        90%
## 0.06594279
```

Then such confidence band for $\mathbb{E}[\hat{p}_h]$ can be used as the confidence band for the persistent homology.

```
##########################################################################
# bootstrap confidence band for persistent homology over a grid
##########################################################################
par(mfrow = c(1,2))
plot(X, xlab = "", ylab = "", main = "Sample X", pch = 20)
plot(x = DiagGrid[["diagram"]], band = 2 * bandKDE[["width"]],
     main = "KDE Diagram")
```



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