Tutorial on the R package TDA

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Abstract

I present a short tutorial and introduction to using the R package **TDA**, which provides tools for Topological Data Analysis. Given data, the sailent topological features of underlying space can be quantified with persistent homology. **TDA** package provides a function for the persistent homology of the Rips filtration, and a function for the persistent homology of sublevel sets (or superlevel sets) of arbitrary functions evaluated over a grid of points. Some common choice of functions for the latter case, such as the distance function, the distance to a measure, the kNN density estimator, the kernel density estimator, and the kernel distance, are implemented in the TDA package. The R package **TDA** also provides a function for computing the confidence band that determines 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. Setting up

Obviously, you should download R first. R of version at least 3.1.0 is recommended:

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/

Before installing R package **TDA**, Four packages are needed to be installed: **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")
}
if (!require(package = "igraph")) {
  install.packages(pkgs = "igraph")
}
if (!require(package = "scales")) {
  install.packages(pkgs = "scales")
}
if (!require(package = "TDA")) {
  install.packages(pkgs = "TDA")
}
```

After that, 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")
}
```

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")
```

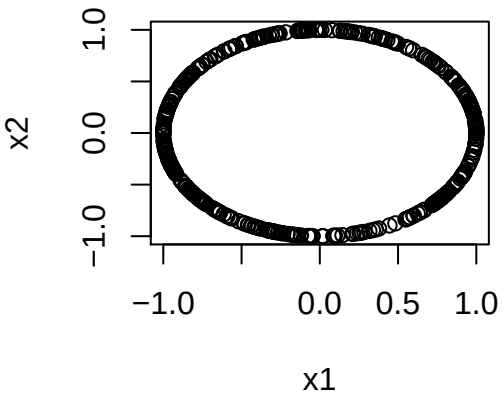
3. Sample on manifolds, Distance Functions, and Density Estimators

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 = 400, r = 1)
plot(circleSample)
```



- n sample from the uniform distribution on the sphere S^d in $\mathbb{R}^{d+1}$ with radius r.

```
################################################################################
# uniform sample on the sphere
################################################################################
sphereSample <- sphereUnif(n = 10000, d = 2, r = 1)
if (!require(package = "rgl")) {
  install.packages(pkgs = "rgl")
}
library(rgl)
plot3d(sphereSample)
```

- n sample from the uniform distribution on the torus in $\mathbb{R}^3$ with small radius a and large radius b.

```
################################################################################
# uniform sample on the torus
################################################################################
```

```
torusSample <- torusUnif(n = 10000, a = 1.8, c = 5)
if (!require(package = "rgl")) {
  install.packages(pkgs = "rgl")
}
library(rgl)
plot3d(torusSample)
```

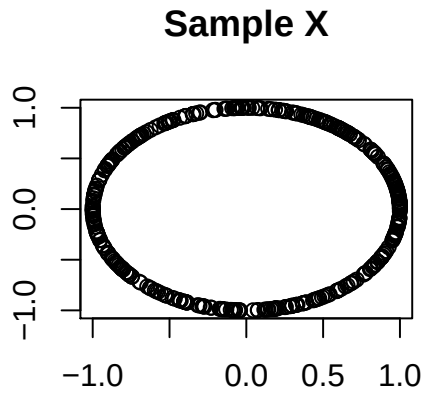
3.2. Distance Functions, and Density Estimators

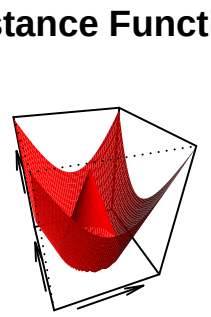
We compute distance functions and density estimators over a grid of points. Suppose a set of points $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ has been sampled from some distribution P. The following code generates a sample of 400 points from the unit circle and constructs a grid of points over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

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

Xlim <- c(-1.6, 1.6)
Ylim <- c(-1.7, 1.7)
by <- 0.065
Xseq <- seq(from = Xlim[1], to = Xlim[2], by = by)
Yseq <- seq(from = Ylim[1], to = Ylim[2], by = by)
Grid <- expand.grid(Xseq, Yseq)
```

- The distance function is defined for each $y \in \mathbb{R}^d$ as $\Delta(y) = \inf_{x \in X} \|x - y\|_2$.

```
################################################################################
# distance function
################################################################################
distance <- distFct(X = X, Grid = Grid)

par(mfrow = c(1,2))
plot(X, xlab = "", ylab = "", main = "Sample X")
persp(x = Xseq, y = Yseq,
      z = matrix(distance, nrow = length(Xseq), ncol = length(Yseq)),
      xlab = "", ylab = "", zlab = "", theta = -20, phi = 35, scale = FALSE,
      expand = 3, col = "red", border = NA, ltheta = 50, shade = 0.5,
      main = "Distance Function")
```





- Given a probability measure P, the distance to measure (DTM) is defined for each $y \in \mathbb{R}^d$ as

$$d_{m_0}(y) = \sqrt{\frac{1}{m_0}\int_0^{m_0}(G_y^{-1}(u))^2 du},$$

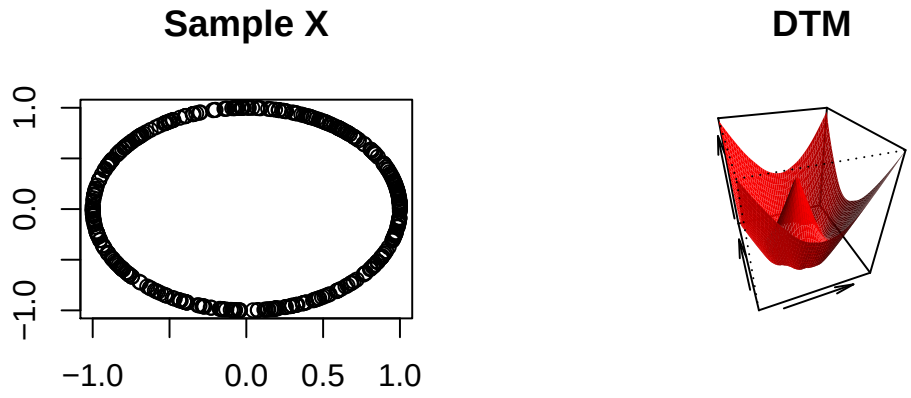
where $G_y(t) = P(\|X - y\| \leq t)$ and $0 < m_0 < 1$ is a smoothing parameter. The DTM can be seen as a smoothed version of the distance function. For more details see **?**.

Given $X = \{x_1, \ldots, x_n\}$, the empirical version of the DTM is

$$\hat{d}_{m_0}(y) = \sqrt{\frac{1}{k}\sum_{x_i \in N_k(y)} \|x_i - y\|^2},$$

where $k = \lceil m_0 n \rceil$ and $N_k(y)$ is the set containing the k nearest neighbors of y among $x_1, \ldots, x_n$.

```
##############################################################################
# distance to measure
##############################################################################
m0 <- 0.1
DTM <- dtm(X = X, Grid = Grid, m0 = m0)

par(mfrow = c(1,2))
plot(X, xlab = "", ylab = "", main = "Sample X")
persp(x = Xseq, y = Yseq,
      z = matrix(DTM, nrow = length(Xseq), ncol = length(Yseq)),
      xlab = "", ylab = "", zlab = "", theta = -20, phi = 35, scale = FALSE,
      expand = 3, col = "red", border = NA, ltheta = 50, shade = 0.5,
      main = "DTM")
```

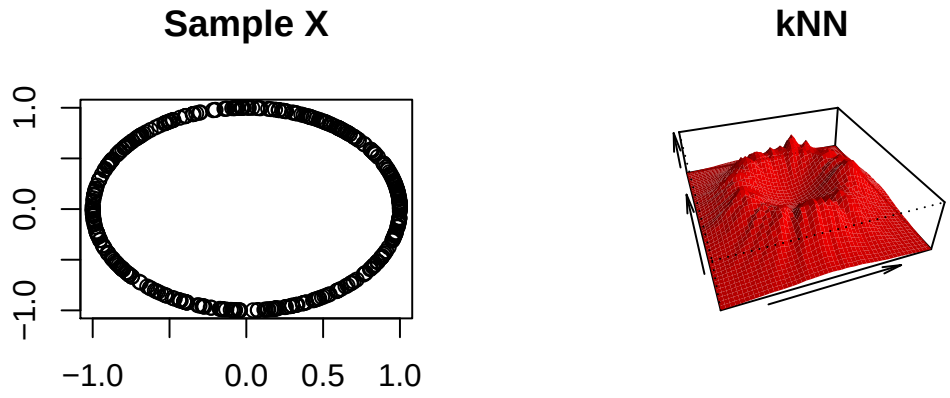


- The k Nearest Neighbor density estimator, for each $y \in \mathbb{R}^d$, is defined as

$$\hat{\delta}_k(y) = \frac{k}{n\, v_d\, r_k^d(y)},$$

where v_n is the volume of the Euclidean d dimensional unit ball and $r_k^d(x)$ is the Euclidean distance form point x to its kth closest neighbor among the points of X.

```
##############################################################################
# k nearest neighbor density estimator
##############################################################################
k <- 60
kNN <- knnDE(X = X, Grid = Grid, k = k)

par(mfrow = c(1,2))
plot(X, xlab = "", ylab = "", main = "Sample X")
persp(x = Xseq, y = Yseq,
      z = matrix(kNN, nrow = length(Xseq), ncol = length(Yseq)),
      xlab = "", ylab = "", zlab = "", theta = -20, phi = 35, scale = FALSE,
      expand = 3, col = "red", border = NA, ltheta = 50, shade = 0.5,
      main = "kNN")
```

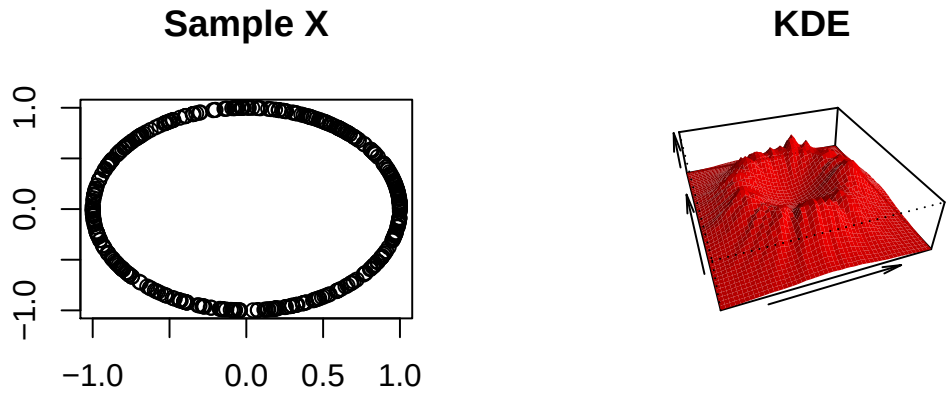


- The Gaussian Kernel Density Estimator (KDE), for each $y \in \mathbb{R}^d$, is defined as

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

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

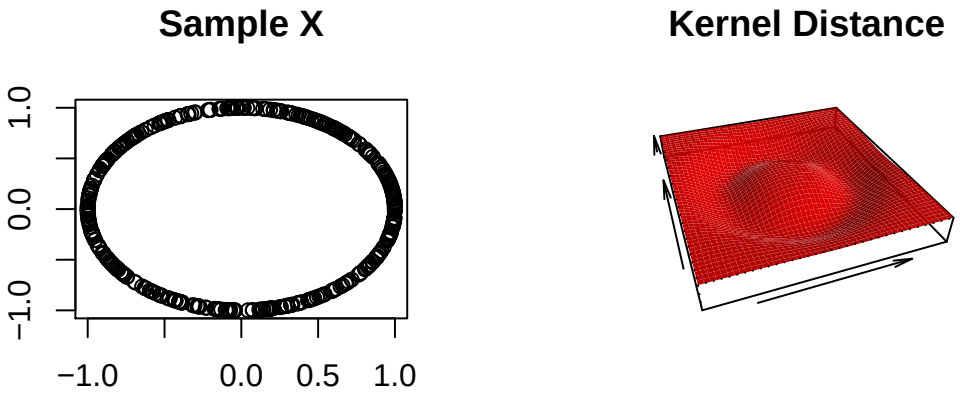


- The Kernel distance estimator, for each $y \in \mathbb{R}^d$, is defined as

$$\hat{\kappa}_h(y) = \sqrt{\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} K_h(x_i, x_j) + K_h(y, y) - 2\frac{1}{n}\sum_{i=1}^{n} K_h(y, x_i)},$$

where $K_h(x, y) = \exp\left(\frac{-\|x-y\|_2^2}{2h^2}\right)$ is the Gaussian Kernel with smoothing parameter h.

```
##############################################################################
# kernel distance
##############################################################################
h <- 0.3
Kdist <- kernelDist(X = X, Grid = Grid, h = h)

par(mfrow = c(1,2))
plot(X, xlab = "", ylab = "", main = "Sample X")
persp(x = Xseq, y = Yseq,
      z = matrix(Kdist, nrow = length(Xseq), ncol = length(Yseq)),
      xlab = "", ylab = "", zlab = "", theta = -20, phi = 35, scale = FALSE,
      expand = 3, col = "red", border = NA, ltheta = 50, shade = 0.5,
      main = "Kernel Distance")
```



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 **Dionysus** library (`library = "Dionysus"`) or the **PHAT** library (`library = "PHAT"`) .

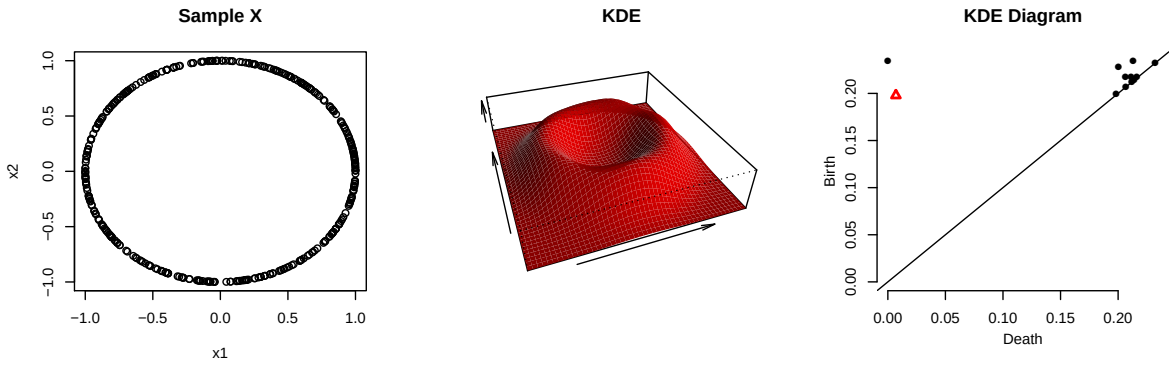
The following code computes the persistent homology of the superlevel sets (`sublevel = FALSE`) of the kernel density estimator (`FUN = kde`, `h = 0.3`) using the point cloud stored in the matrix `X` from the previous example. The other inputs are the features of the grid over which the `kde` is evaluated (`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
###########################################################################
Diag <- gridDiag(X = X, FUN = kde, lim = cbind(Xlim, Ylim), by = by,
    sublevel = FALSE, library = "Dionysus", printProgress = FALSE, h = 0.3)
```

The function `plot` plots persistence diagram for objects of the class `"diagram"`. 8th line of the following command produces the third of the following plot.

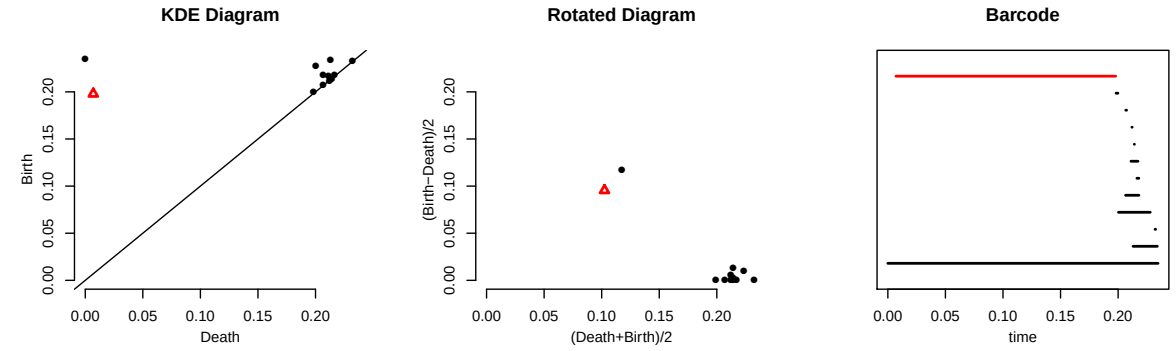
```
###########################################################################
# plotting persistence diagram
###########################################################################
par(mfrow = c(1,3))
plot(X, main = "Sample X")
persp(x = Xseq, y = Yseq,
```

```
      z = matrix(KDE, nrow = length(Xseq), ncol = length(Yseq)),
      xlab = "", ylab = "", zlab = "", theta = -20, phi = 35, scale = FALSE,
      expand = 3, col = "red", border = NA, ltheta = 50, shade = 0.9,
      main = "KDE")
plot(x = Diag[["diagram"]], main = "KDE Diagram")
```



The function `plot` for the class `"diagram"` provide the options of rotating the diagram (`rotated = TRUE`), drawing the barcode in place of the diagram (`barcode = TRUE`).

```
#############################################################################
# other options for plotting persistence diagram
#############################################################################
par(mfrow = c(1,3))
plot(Diag[["diagram"]], main = "KDE Diagram")
plot(Diag[["diagram"]], rotated = TRUE, main = "Rotated Diagram")
plot(Diag[["diagram"]], barcode = TRUE, main = "Barcode")
```

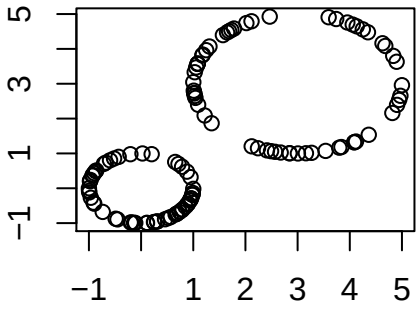


4.2. Rips Diagrams

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. 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 persistence diagram using either the C++ library **GUDHI** (`library = "GUDHI"`) , or **Dionysus** (`library = "Dionysus"`) .

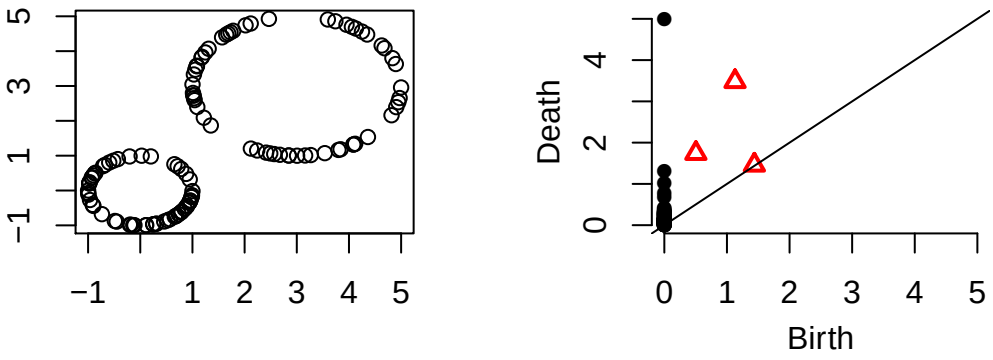
The following code generates 60 points from two circles, as in the following figure:

```
#############################################################################
# generating samples from two circles
#############################################################################
Circle1 <- circleUnif(n = 60)
Circle2 <- circleUnif(n = 60, r = 2) + 3
Circles <- rbind(Circle1, Circle2)
plot(Circles, xlab="", ylab="")
```



We specify the limit of the Rips filtration(maxscale = 5) and the max dimension(maxdimension = 1) of the homological features we are interested in (0 for components, 1 for loops, 2 for voids, etc.). Then we plot the data and the diagram.

```
#############################################################################
# Rips persistence diagram
#############################################################################
Diag <- ripsDiag(X = Circles, maxdimension = 1, maxscale = 5,
    library = "GUDHI", printProgress = FALSE)
par(mfrow=c(1,2))
plot(Circles, xlab="", ylab="")
plot(Diag[["diagram"]])
```

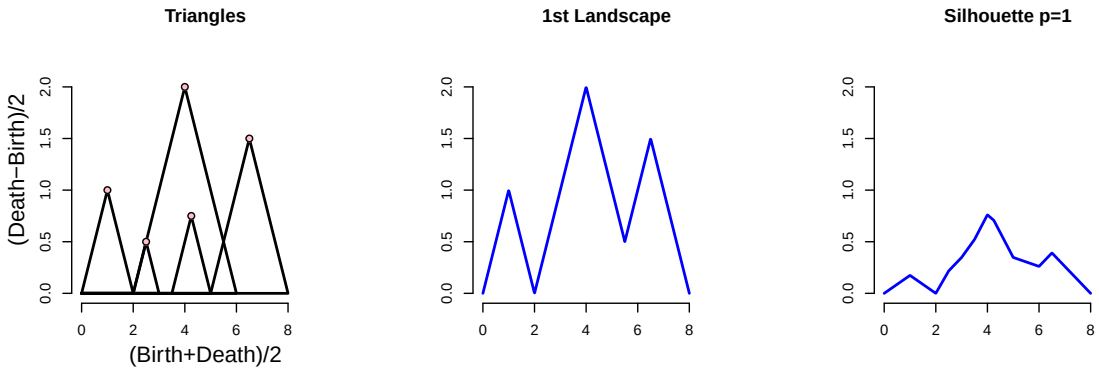


4.3. Bottleneck and Wasserstein Distances

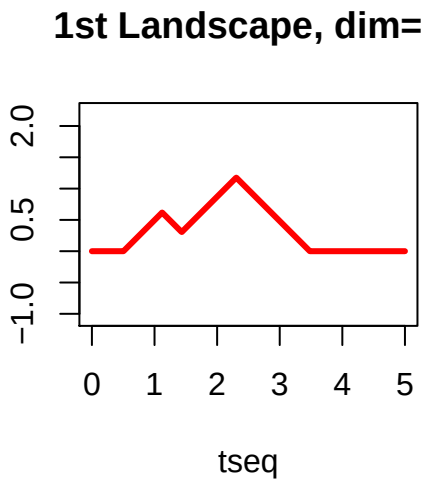
```
Diag1 <- ripsDiag(X = Circle1, maxdimension = 1, maxscale = 5)
Diag2 <- ripsDiag(X = Circle2, maxdimension = 1, maxscale = 5)
```

```
print(bottleneck(Diag1 = Diag1[["diagram"]], Diag2 = Diag2[["diagram"]],
    dimension = 1))

## [1] 1.175885

print(wasserstein(Diag1 = Diag1[["diagram"]], Diag2 = Diag2[["diagram"]],
    p = 2, dimension = 1))

## [1] 1.764362
```

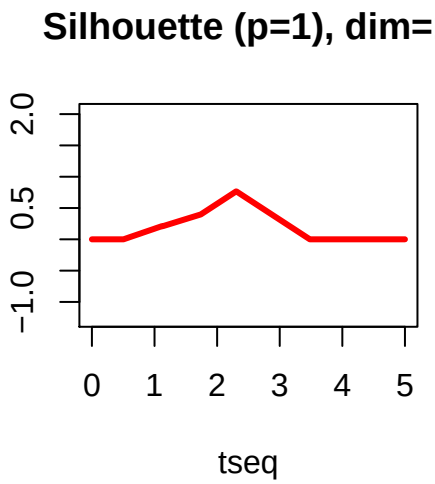
4.4. Landscapes and Silhouettes



```
tseq <- seq(from = 0, to = 5, length = 1000)   #domain
Land <- landscape(Diag = Diag[["diagram"]], dimension = 1, KK = 1, tseq = tseq)
plot(tseq, Land, type = "l", main = "1st Landscape, dim=1", ylab = "", asp = 1,
     col = "red", lwd = 3)
```




```
tseq <- seq(from = 0, to = 5, length = 1000)   #domain
Sil <- silhouette(Diag = Diag[["diagram"]], p = 1,  dimension = 1, tseq = tseq)
plot(tseq, Sil, type = "l", main="Silhouette (p=1), dim=1", ylab = "", asp = 1,
     col = "red", lwd = 3)
```



Affiliation:

Firstname Lastname
Affiliation

Address, Country
E-mail: name@address
URL: http://link/to/webpage/