A statistical approach to algebraic topology

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(joint work with Peter Kim)

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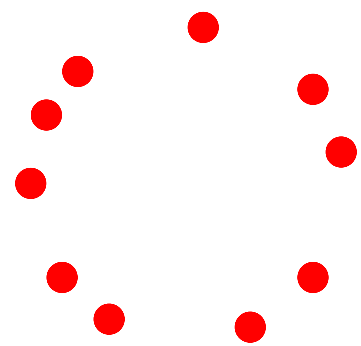
1. Point Cloud Data from densities

Motivation: Given a set of points that "looks like a circle"



We would like to be able to say so mathematically.

Prior and current work

Background: Given a sample, techniques have been developed which detect topological features and give a rough measure of their 'size'.

Our goal: We aim to apply statistical techniques to provide some theoretical rigour to these largely experimental tools. We want to

- given a parameter, calculate expectations of the topological features detected from a sample
- apply bootstrapping to the study of these features

The setting

Given a manifold $\mathbb{M}$ and a (Radon) measure ν, a (probability) density is a function $f : \mathbb{M} \to [0, \infty]$ such that $\int_{\mathbb{M}} f \, d\nu = 1$.

We assume that we have a family of densities

$$\{f_\theta \mid \theta \in \Theta\}$$

where θ is called the parameter and Θ is the parameter space.

In our examples $(\mathbb{M}, \nu)$ is a sphere with spherical measure and Θ is a subset of a finite dimensional vector space.

Point Cloud Data

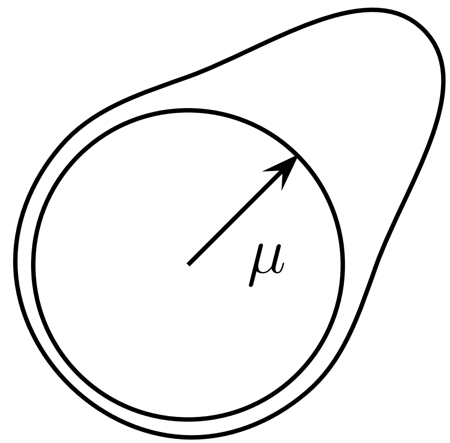
A sample $X_1, X_2, \ldots X_N$ is a sequence of independent and identically distributed random quantities on $\mathbb{M}$ drawn according to the density f_ϑ for some fixed but unknown $\vartheta \in \Theta$.

This sample is called Point Cloud Data (PCD).

We will show that from this PCD one can construct a Rips complex to which one can apply persistent homology to determine Betti barcodes.

Densities on S^1

We will focus on unimodal densities on S^1, called von Mises distributions.



$$f_{\mu,\kappa}(x) = c(\kappa)e^{\kappa x^t \mu}.$$

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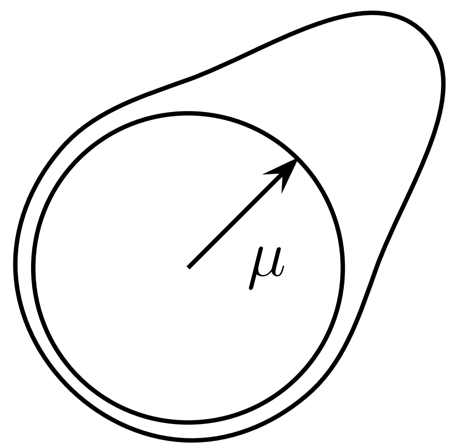
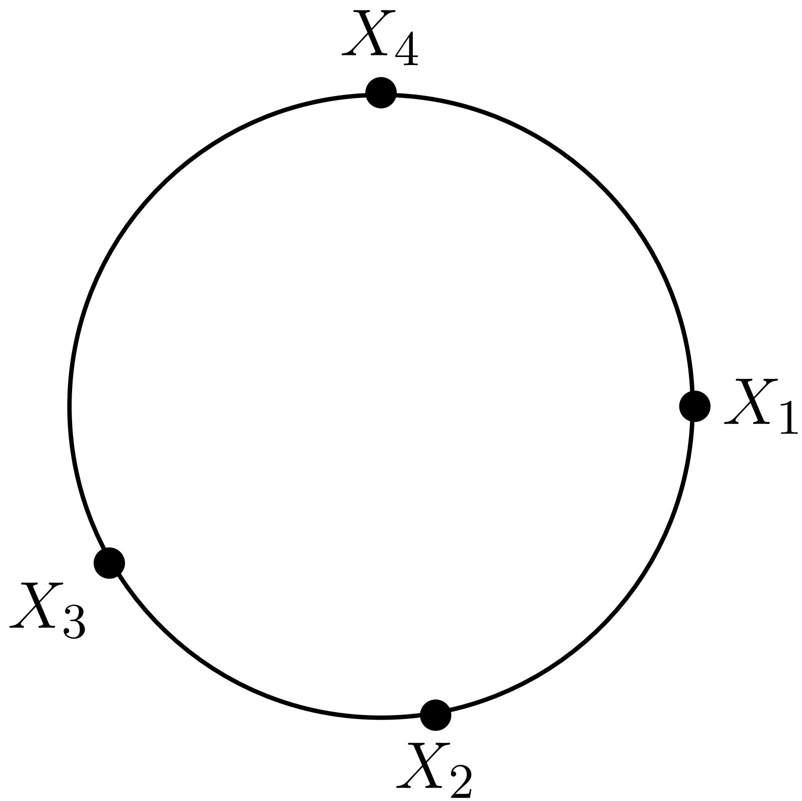


$$f_{\mu,\kappa}(x) = c(\kappa)e^{\kappa x^t \mu}.$$

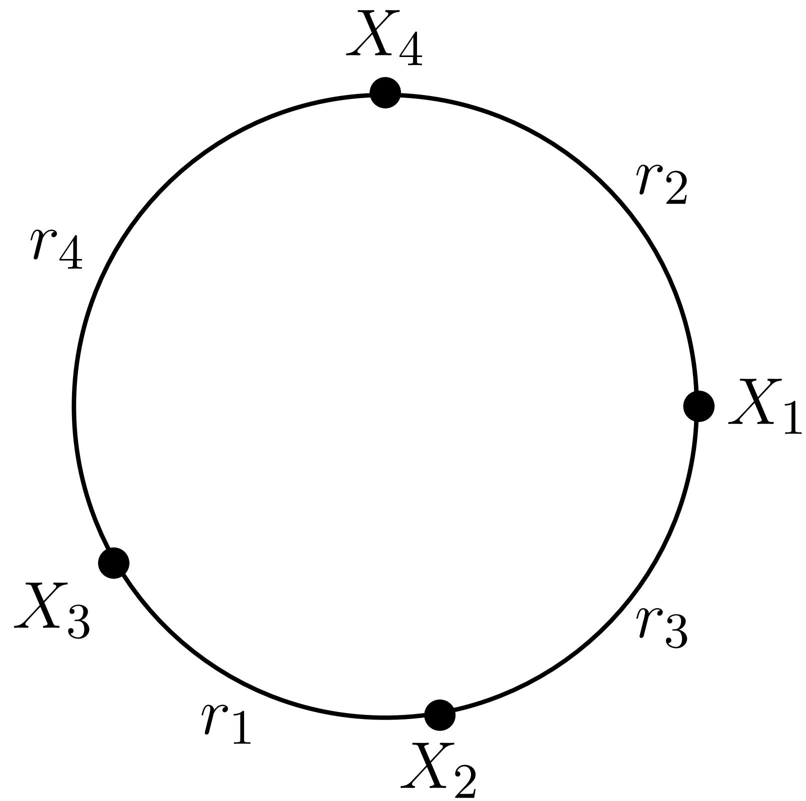
Plan: Sample $X = (X_1, \ldots, X_n) \subset S^1$ according to $f_{\mu,\kappa}$

Construct Rips complex $\xrightarrow{\text{persistent homology}}$ Betti barcodes

2. The Rips complex



2. The Rips complex



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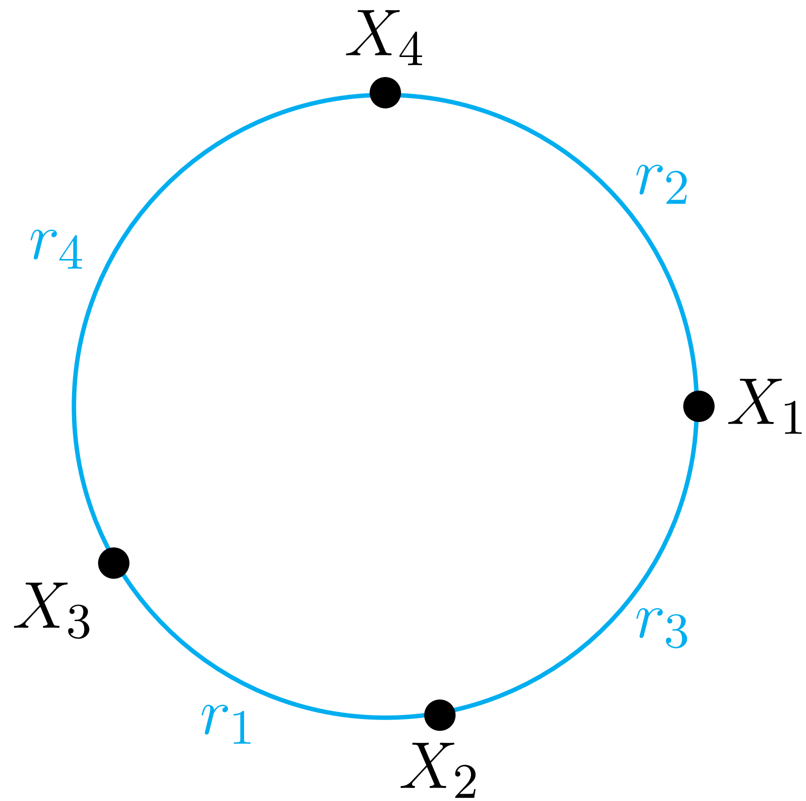

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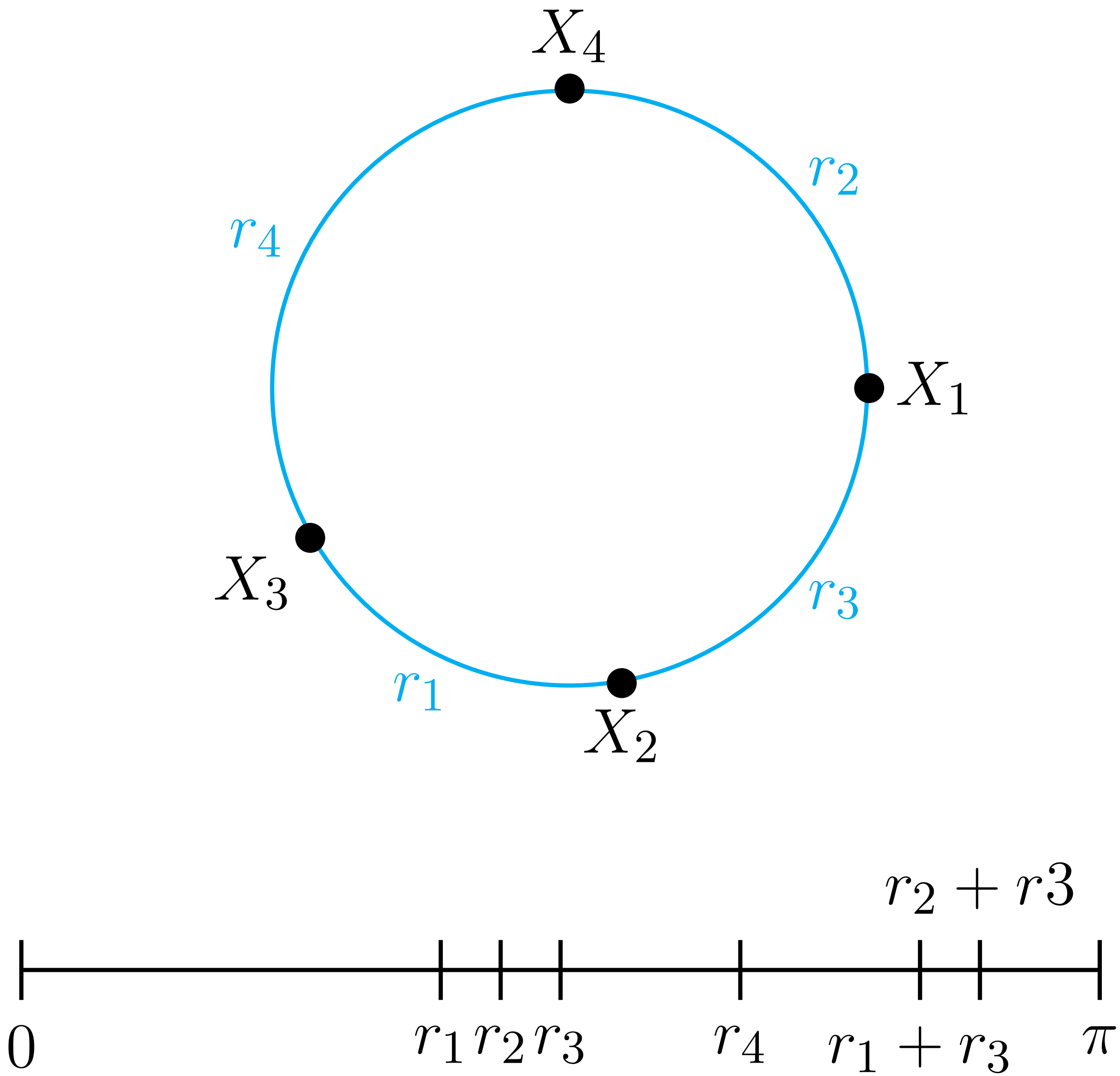

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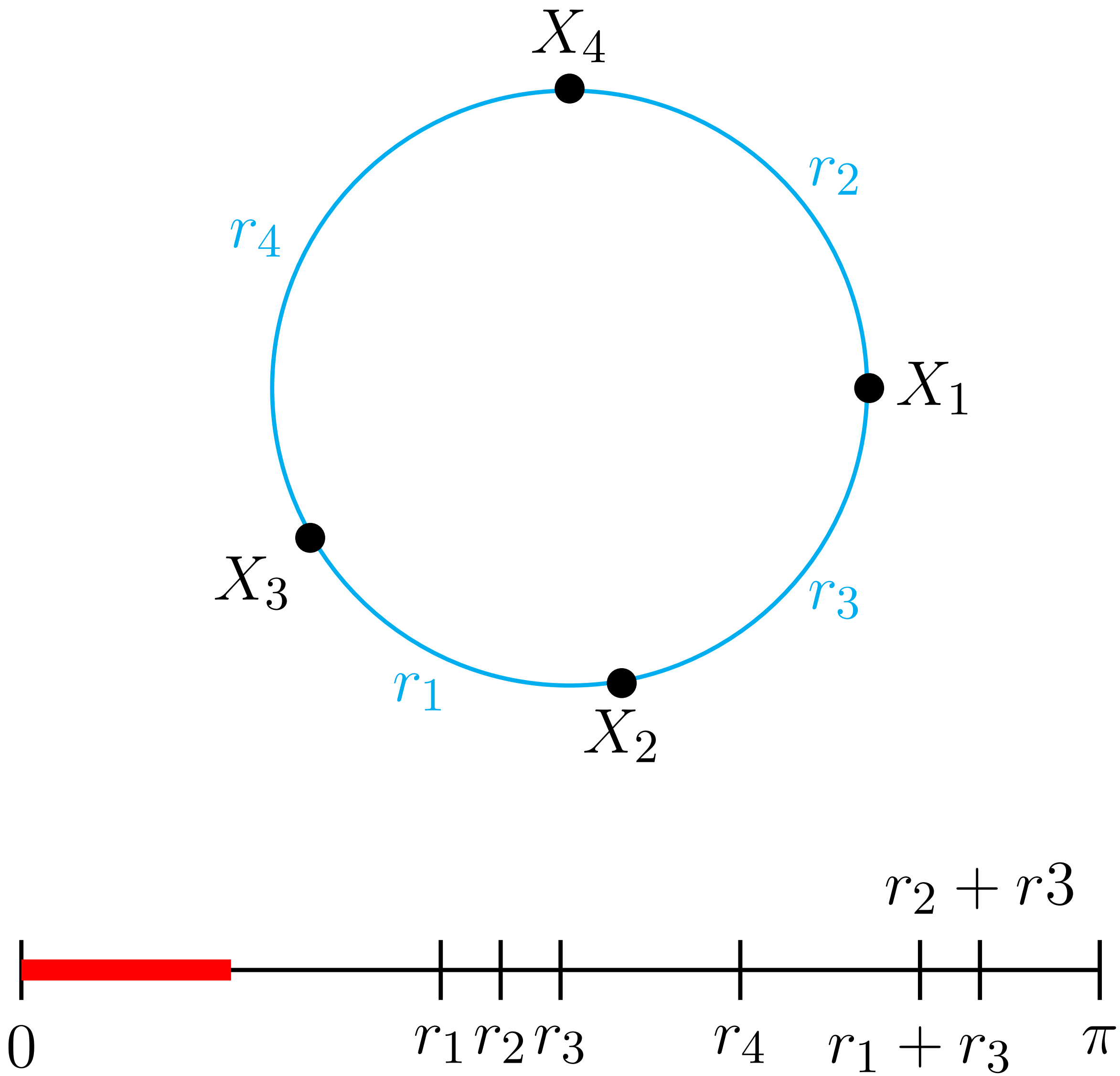

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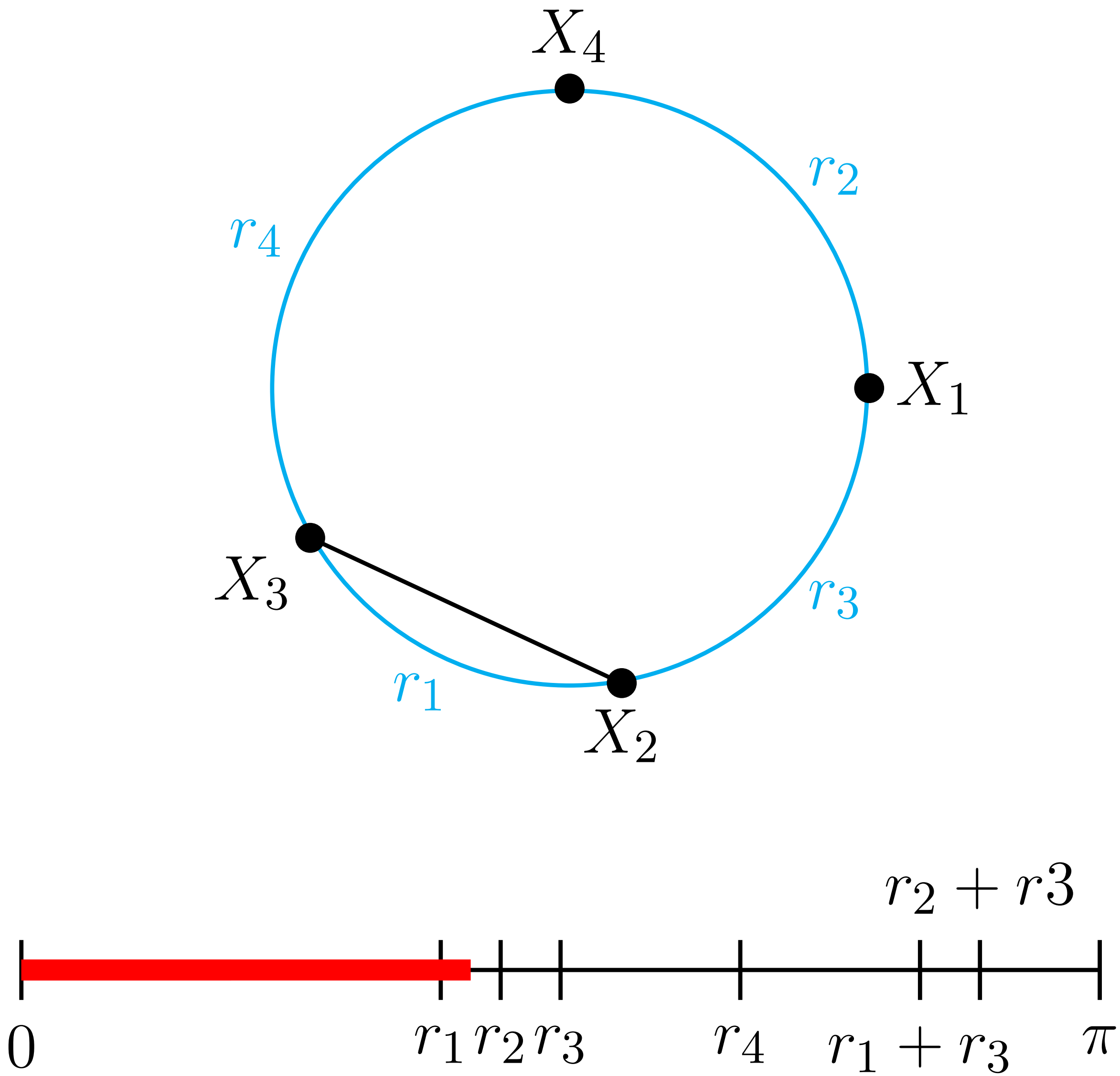

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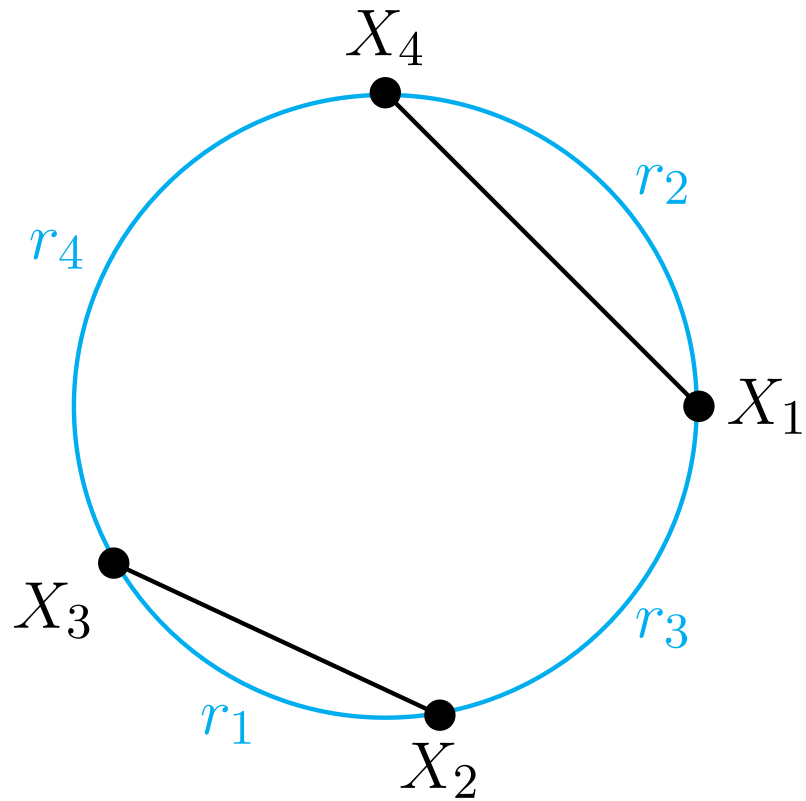

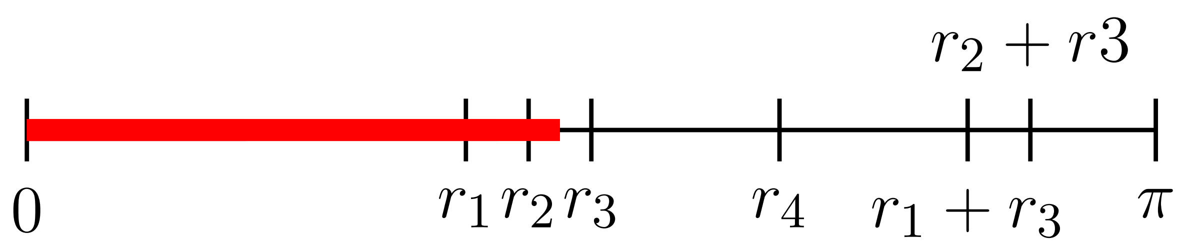

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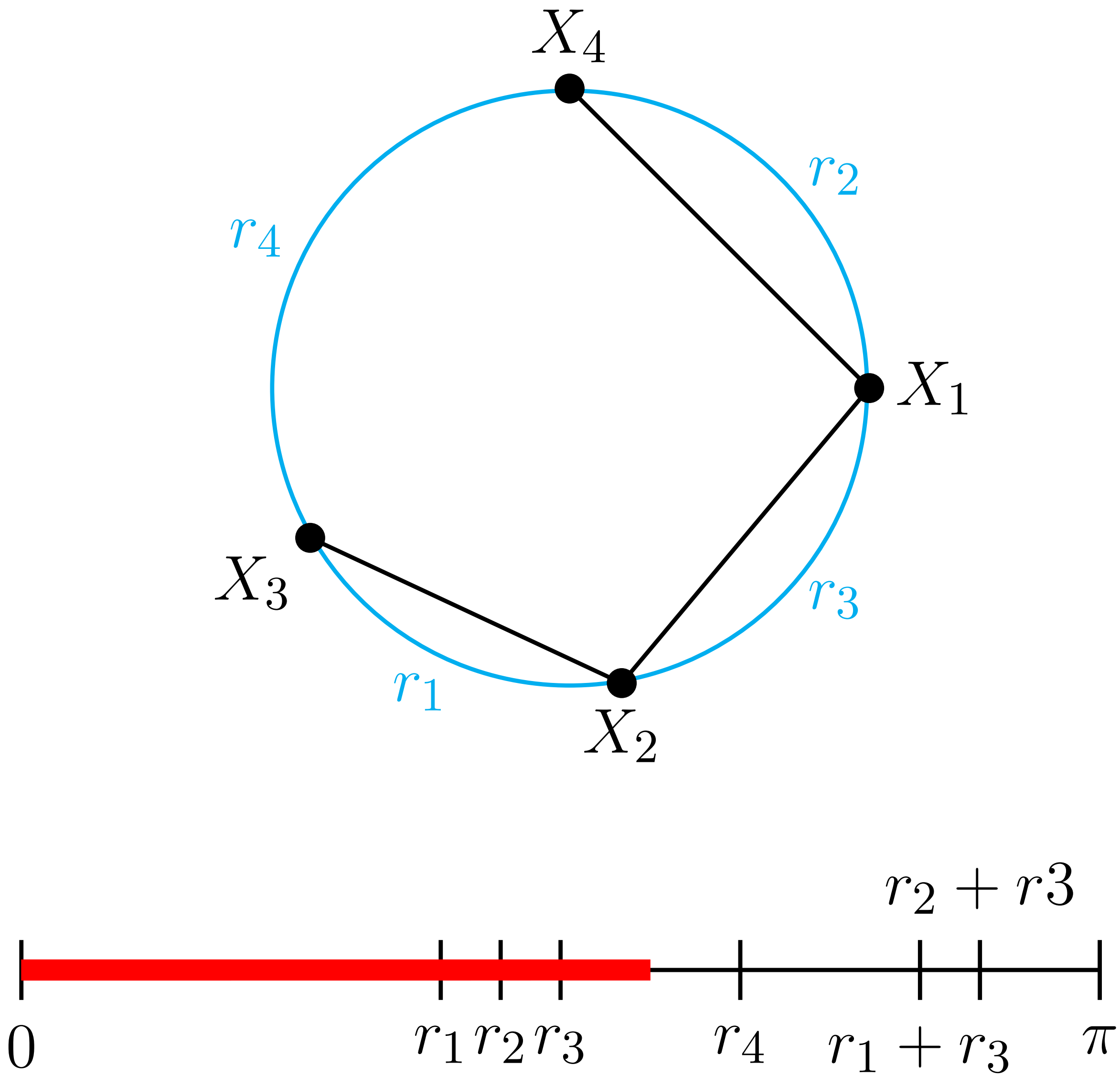

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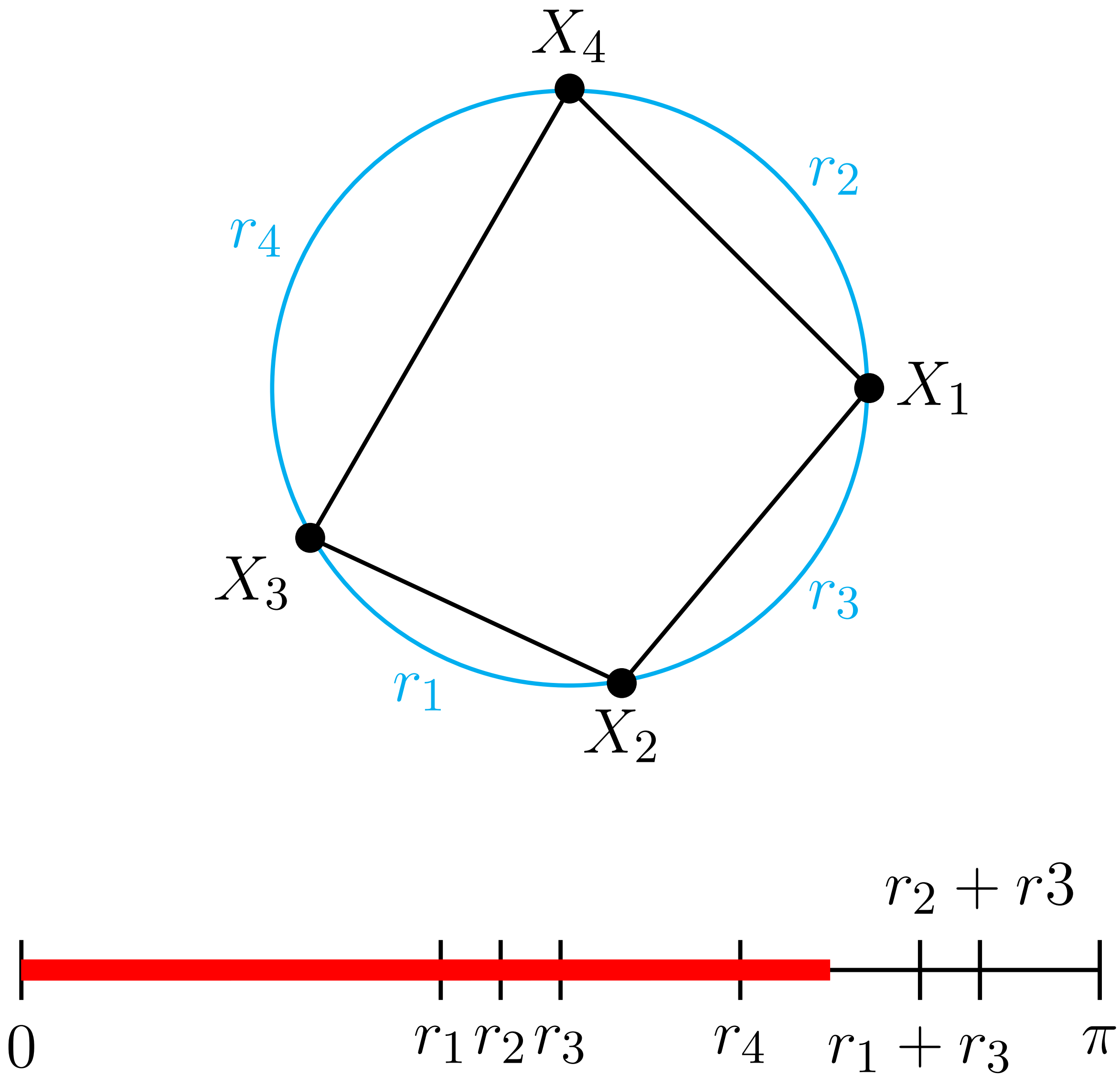

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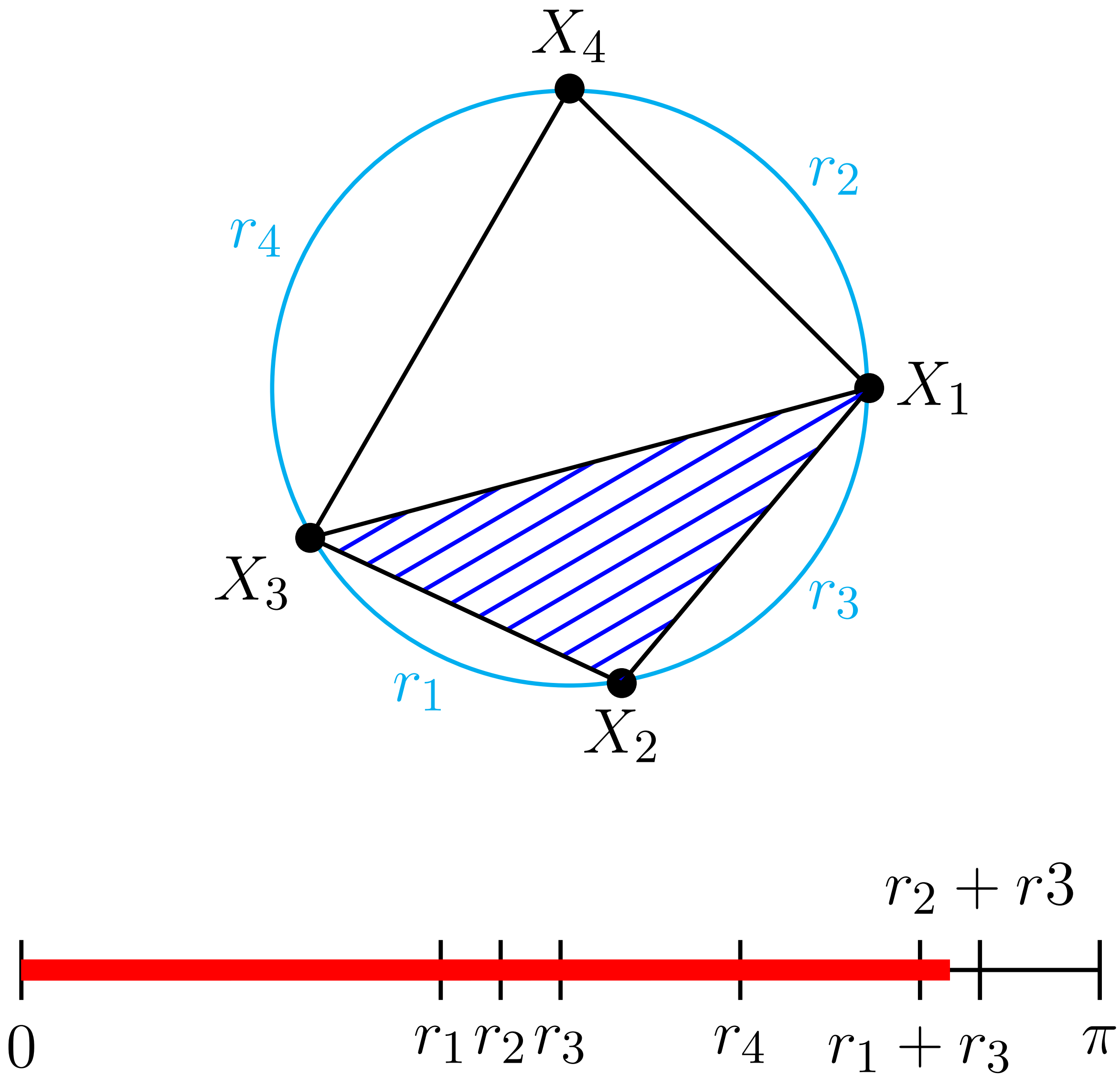

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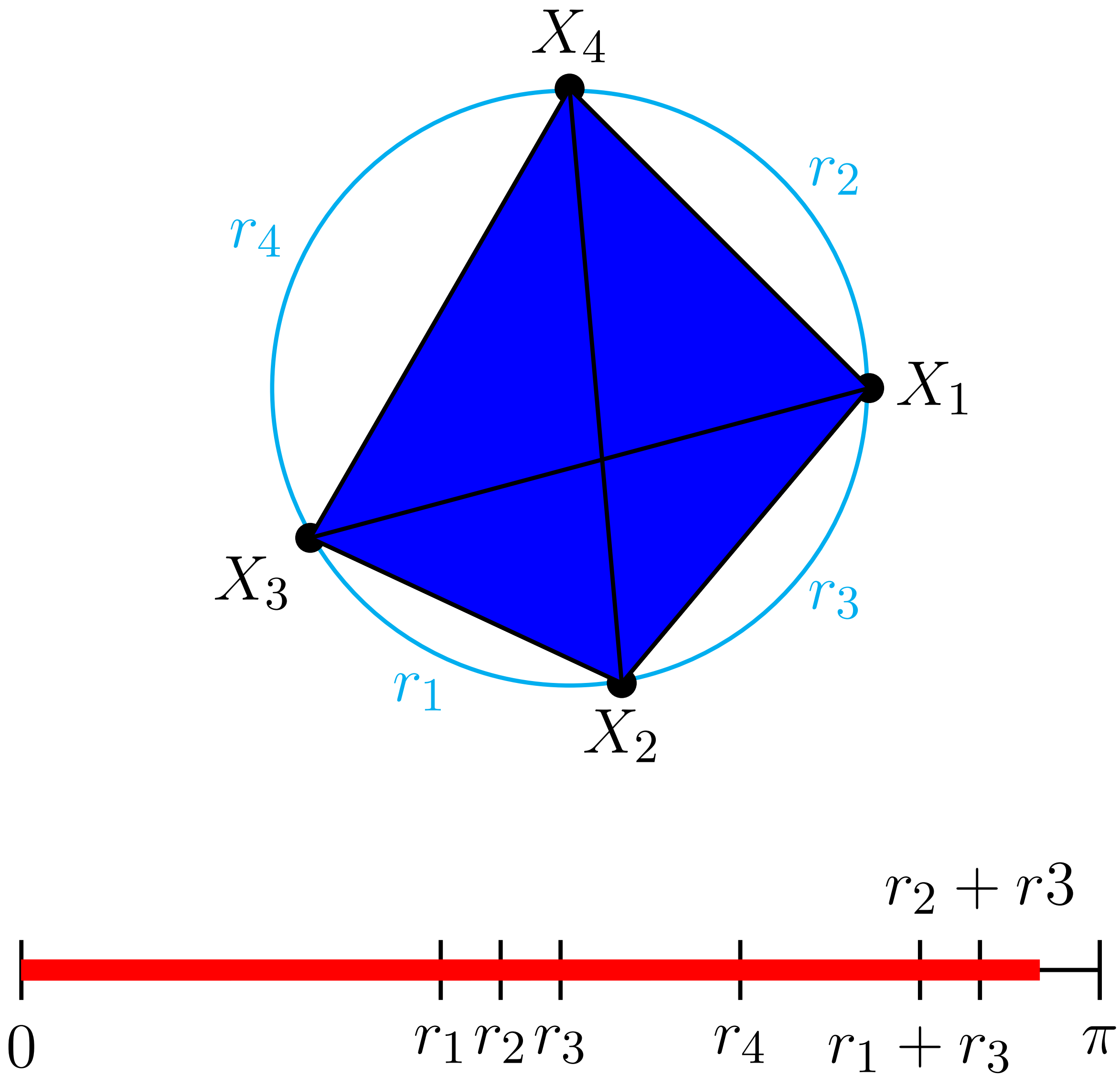
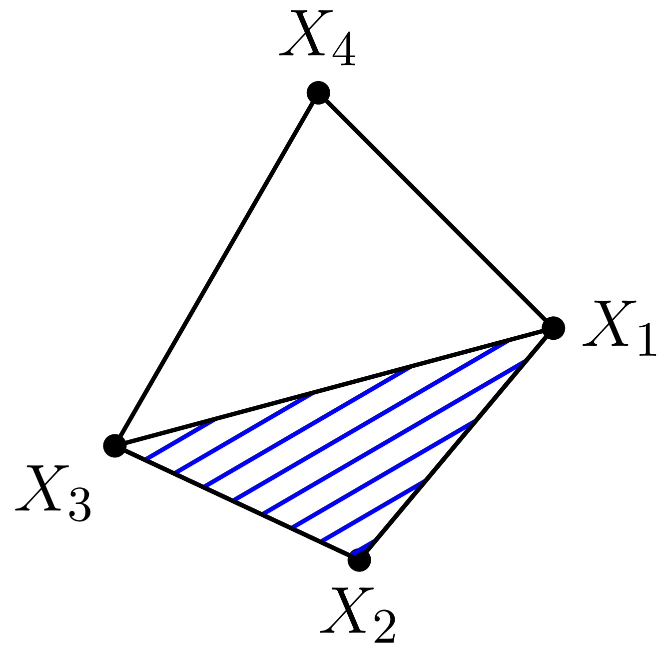


3. Homology of Simplices

Consider the following simplicial complex Δ:

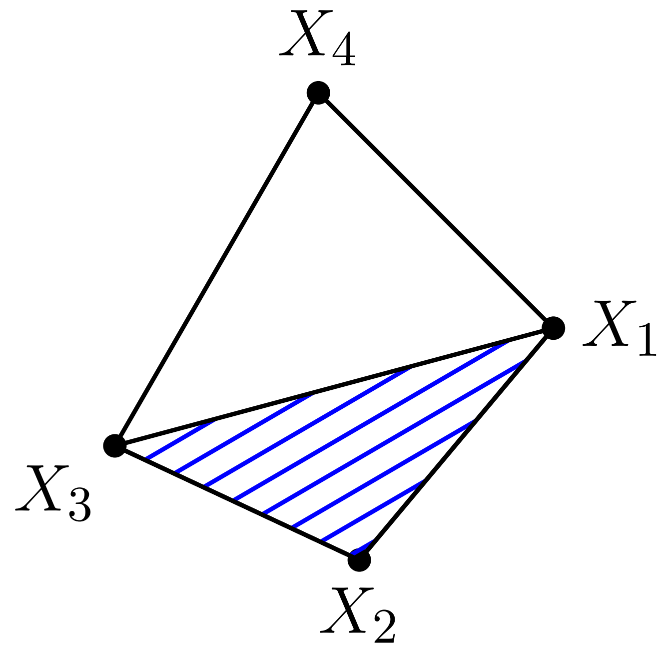


It consists of

- four 0-simplices: X_1, X_2, X_3, X_4,
- five 1-simplicies: $\{X_1, X_2\}$, $\{X_1, X_3\}$, $\{X_2, X_3\}$, $\{X_1, X_4\}$, $\{X_3, X_4\}$,
- and one 2-simplex: $\{X_1, X_2, X_3\}$.

Homology of Simplicies

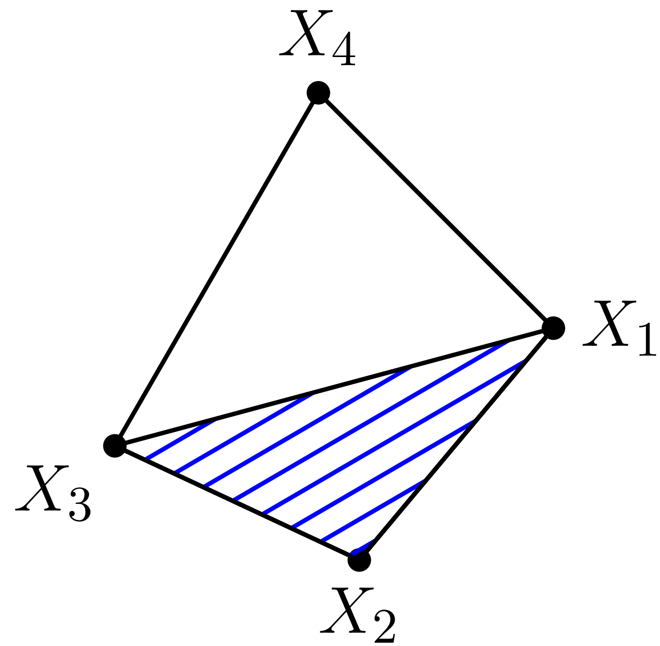
Sums of n-simplicies are called n-chains.



- the boundary of $\{X_1, X_2, X_3\}$ is $\{X_1, X_2\} + \{X_2, X_3\} + \{X_3, X_1\}$
- the boundary of $\{X_i, X_j\}$ is $X_j - X_i$,
- the boundary of $\{X_i\}$ is 0

Homology of Simplicies

By linearity this defines the boundary on all n-chains.



Cycles are n-chains with boundary equal to zero.

For example $\{X_1, X_2\} + \{X_2, X_3\} + \{X_3, X_1\}$ is a cycle and so is X_1.

One can check that boundaries are always cycles.

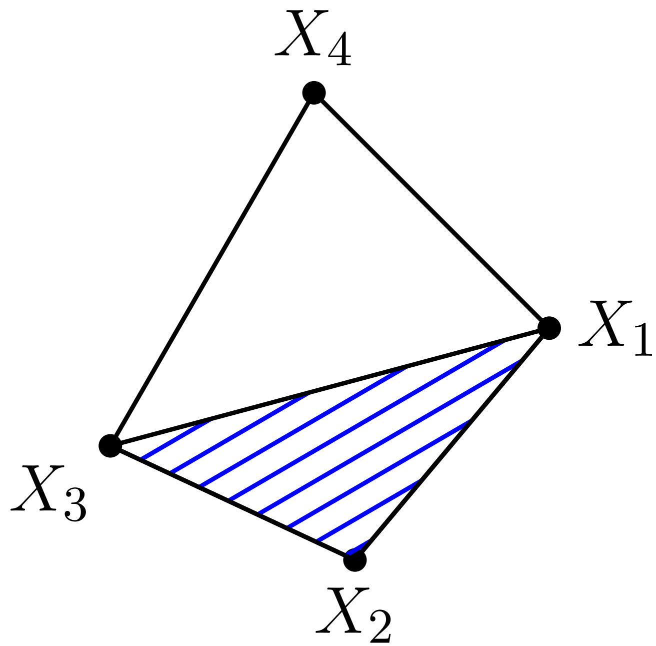
Homology of Simplicies

The homology $H_n(\Delta)$ is the quotient of the cycles modulo the boundaries.

The Betti number $B_n(\Delta)$ is the dimension of $H_n(\Delta)$.

$B_0(\Delta)$ is the number of connected components of Δ.
$B_1(\Delta)$ is the number of holes in Δ.
$B_2(\Delta)$ is the number of voids in Δ.

Homology of Simplicies



In our example $B_0(\Delta) = 1$, $B_1(\Delta) = 1$, and all higher Betti numbers are zero.

4. Persistent homology

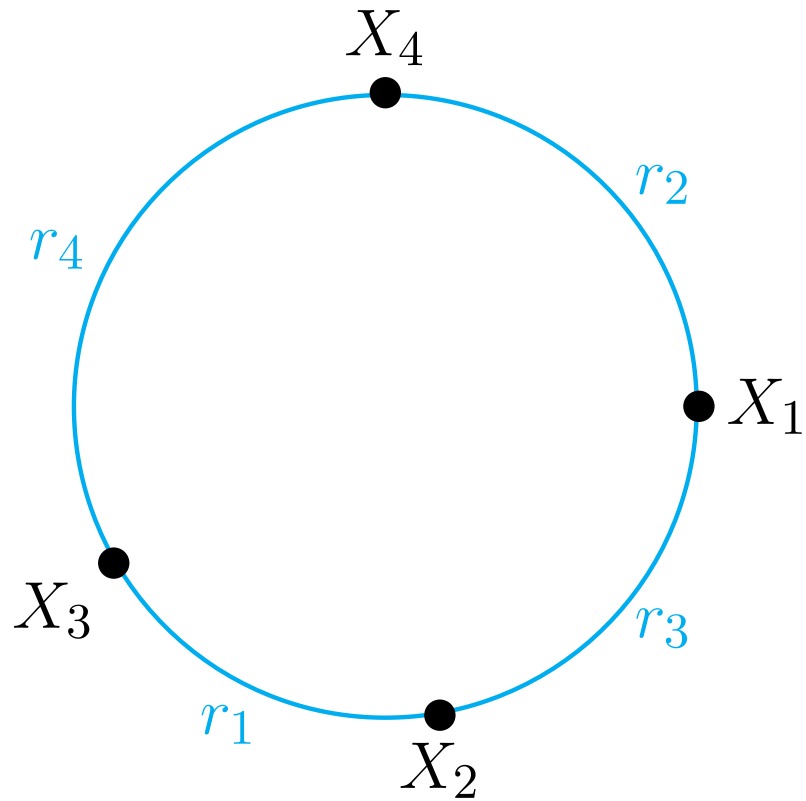
Assume we have a simplicial complex that changes as we vary some parameter r.

The homology that persists as r changes is called persistent homology.

We can record how the Betti numbers change as r changes using Betti barcodes.

We illustrate this using the Rips complex on our earlier example.

The Rips complex



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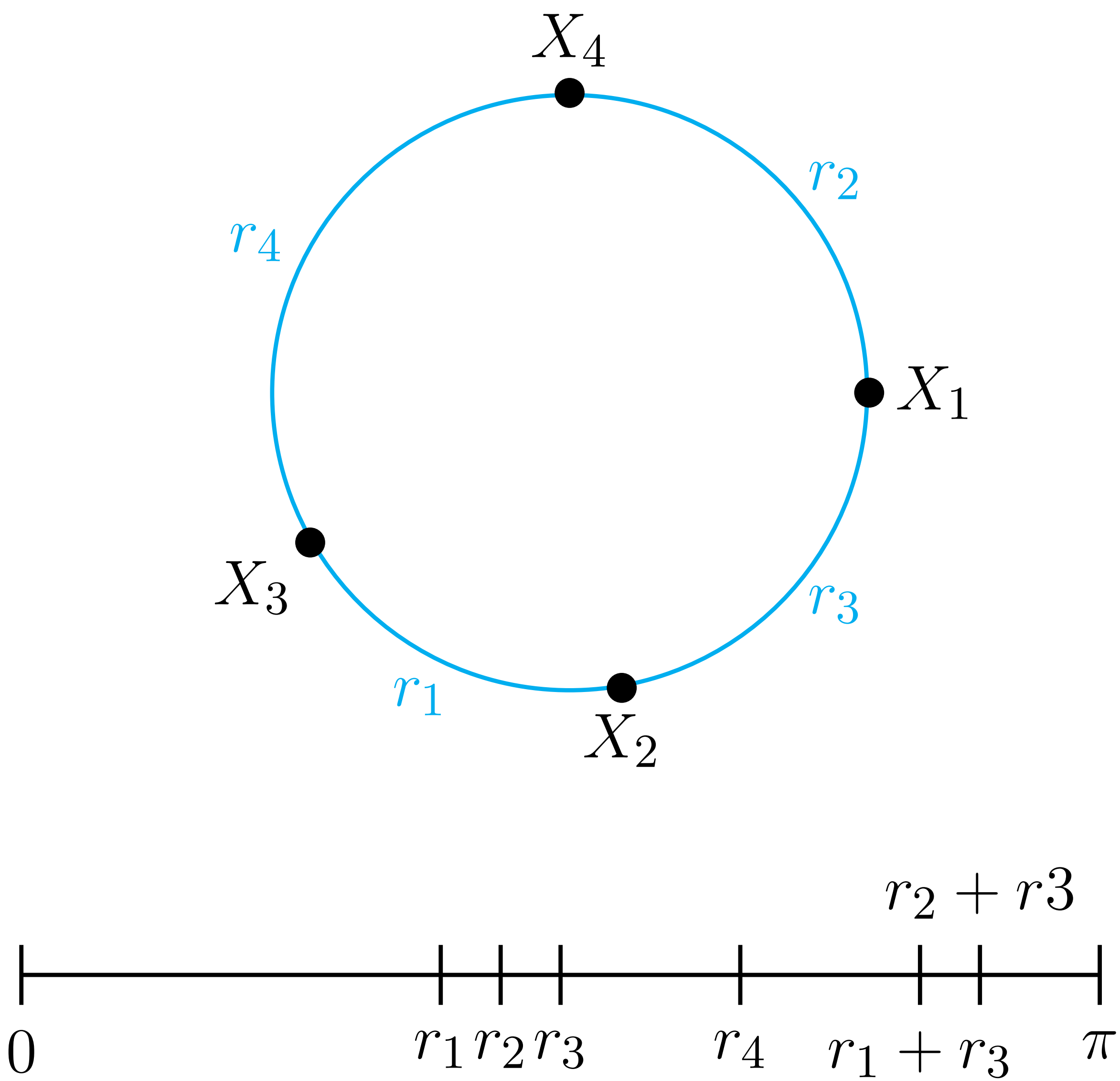

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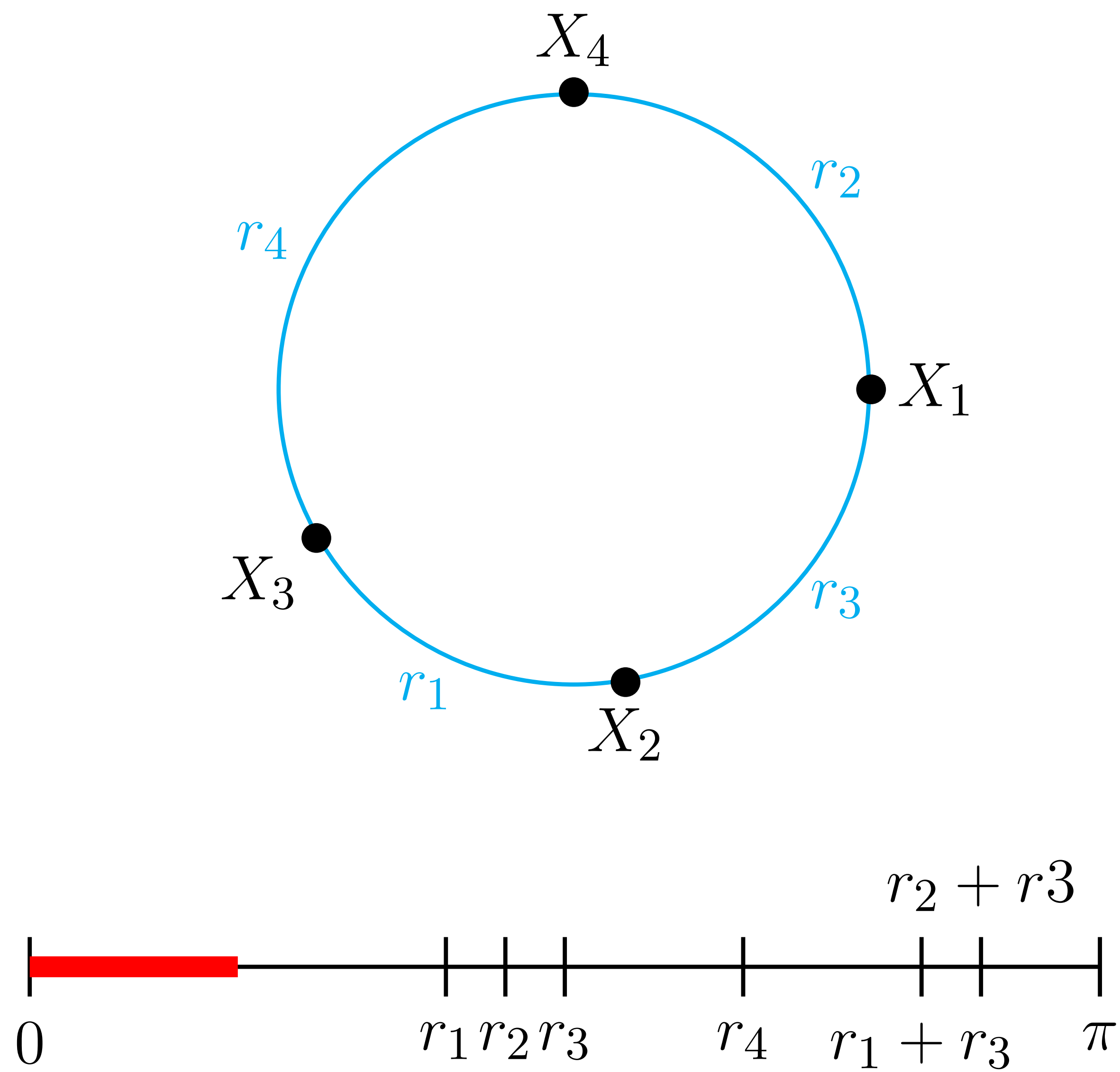

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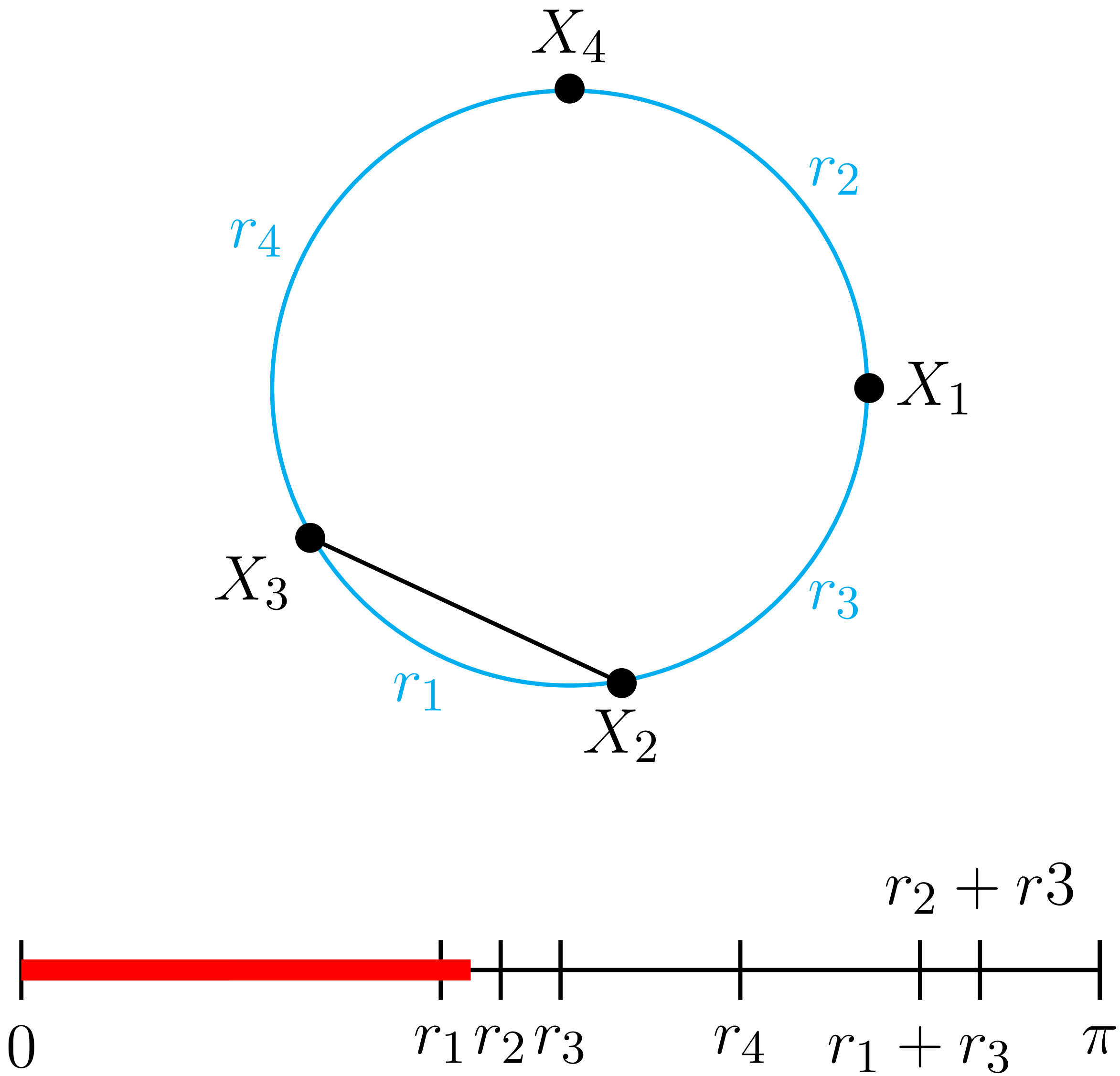

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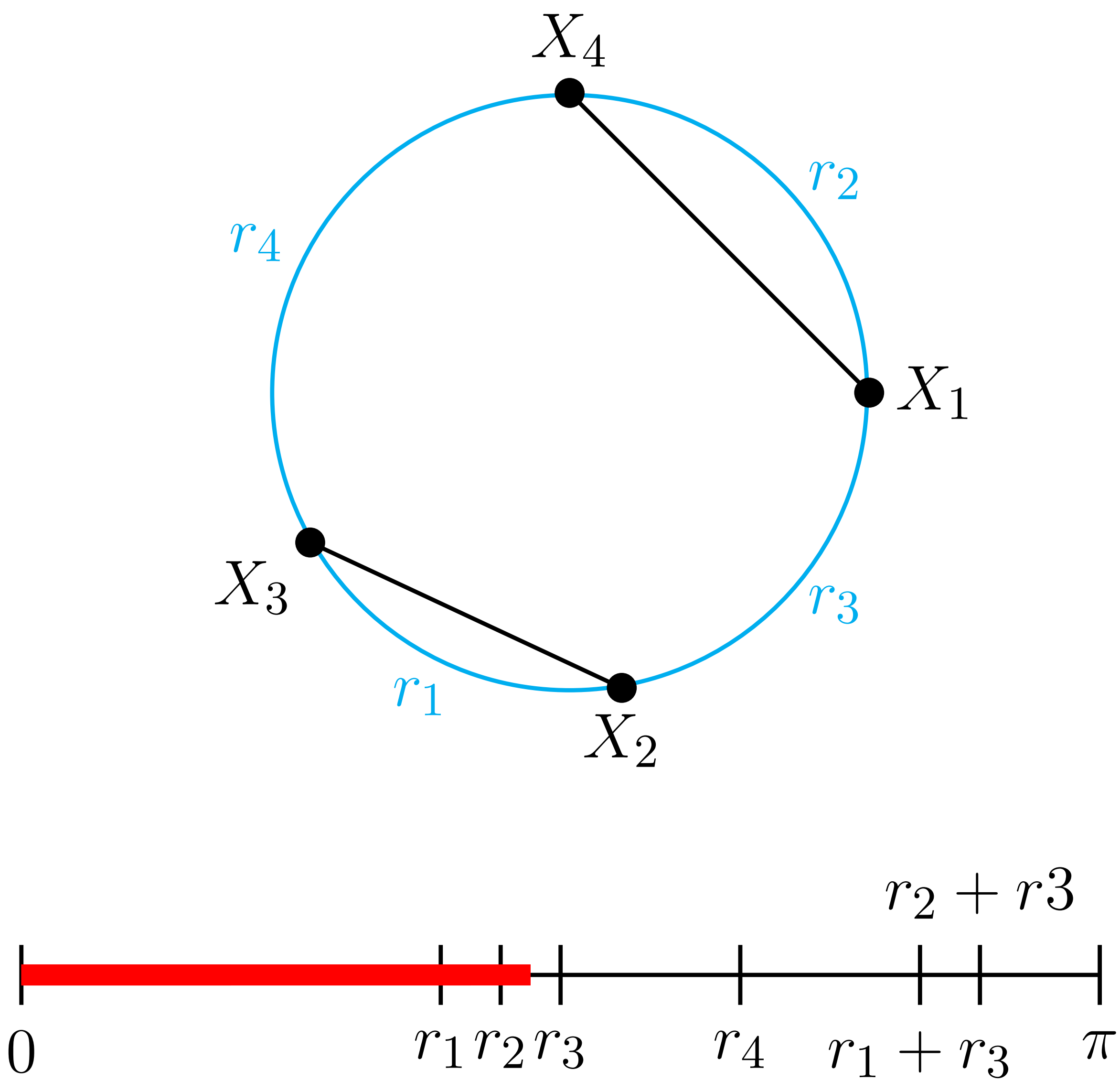

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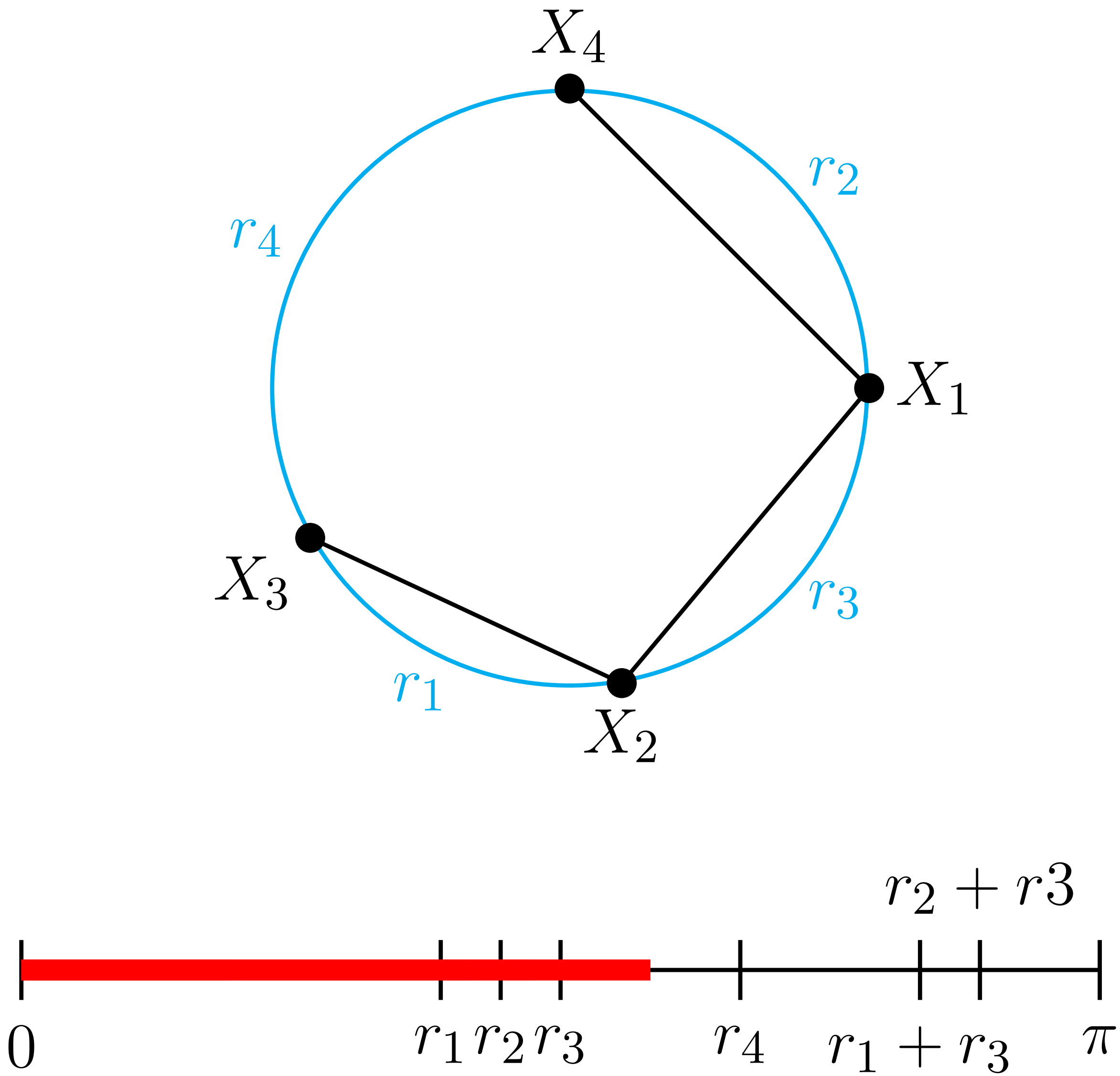

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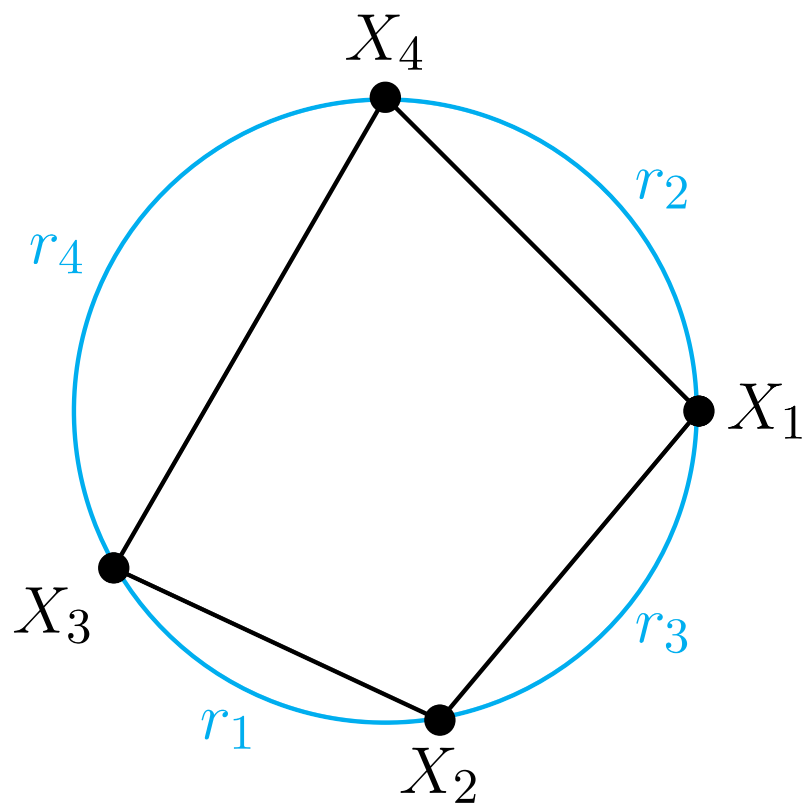

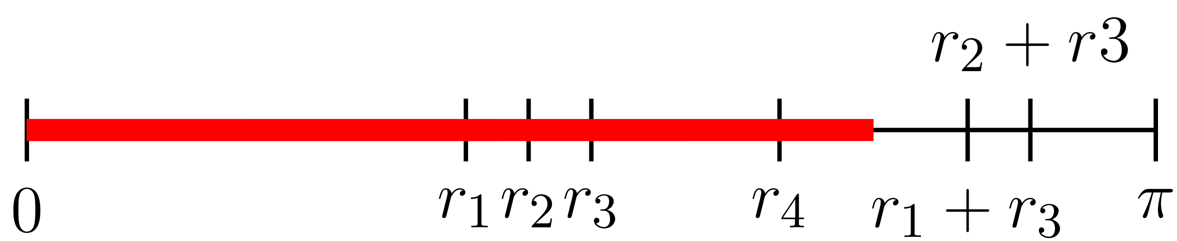

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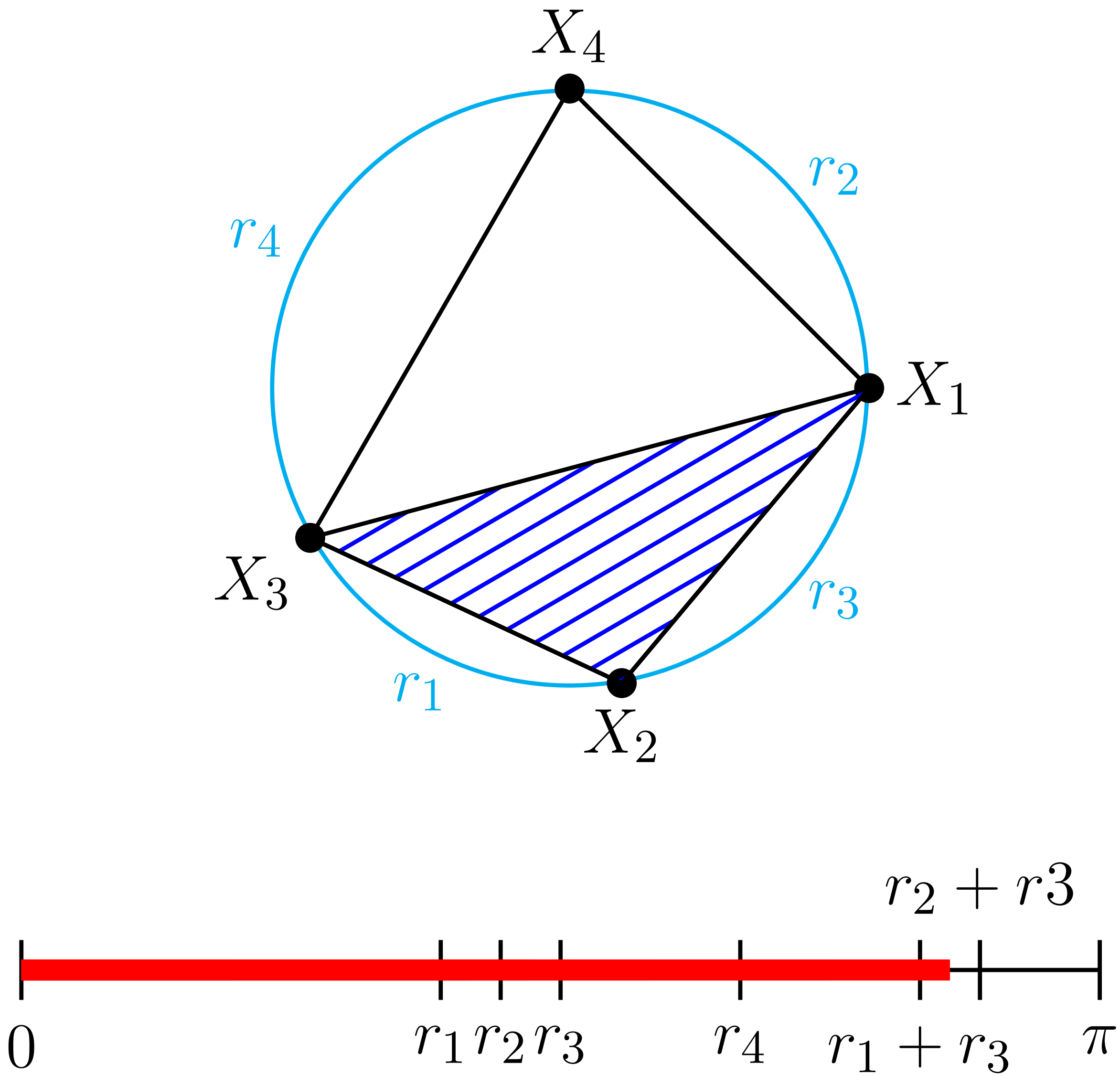

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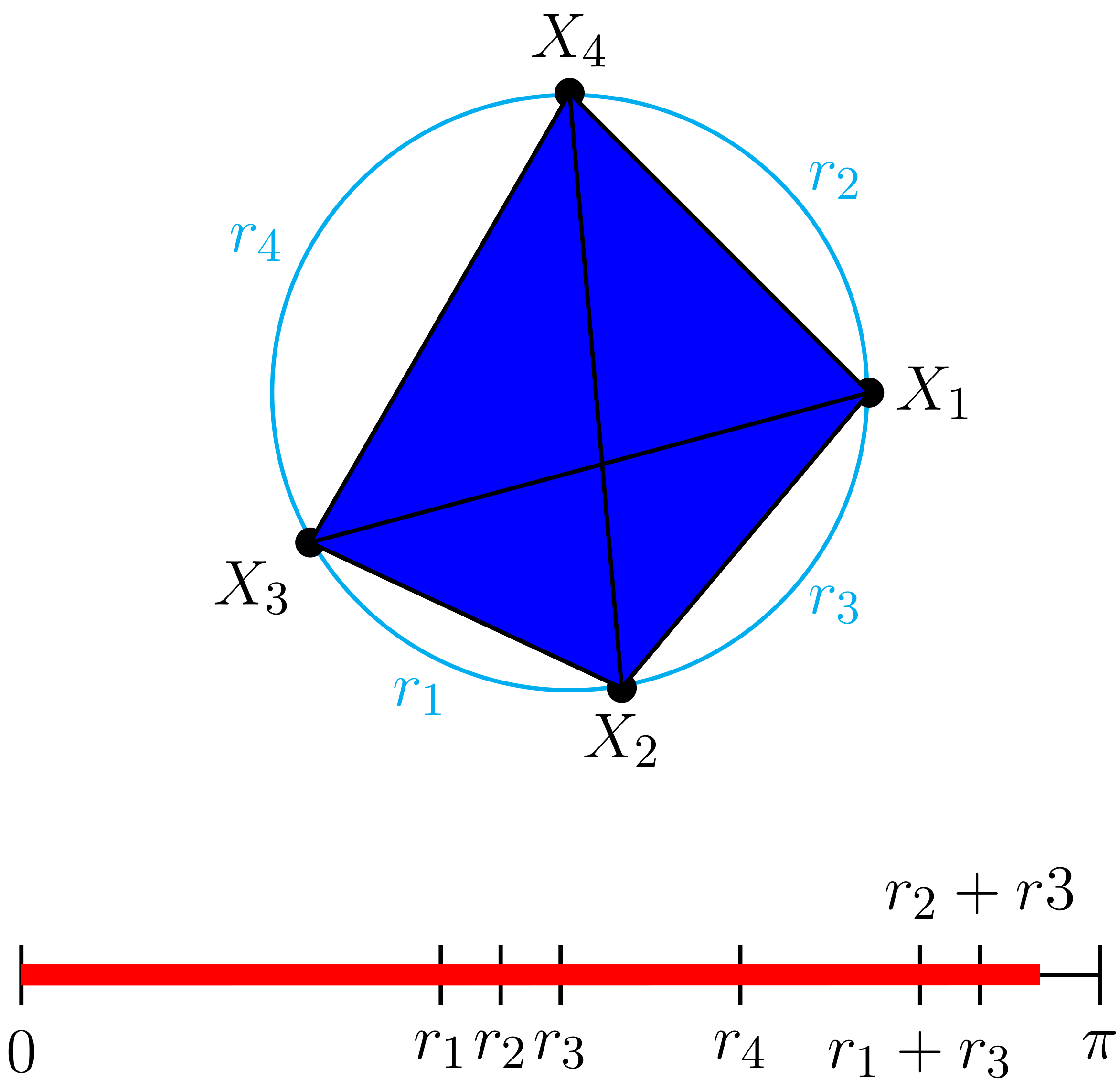
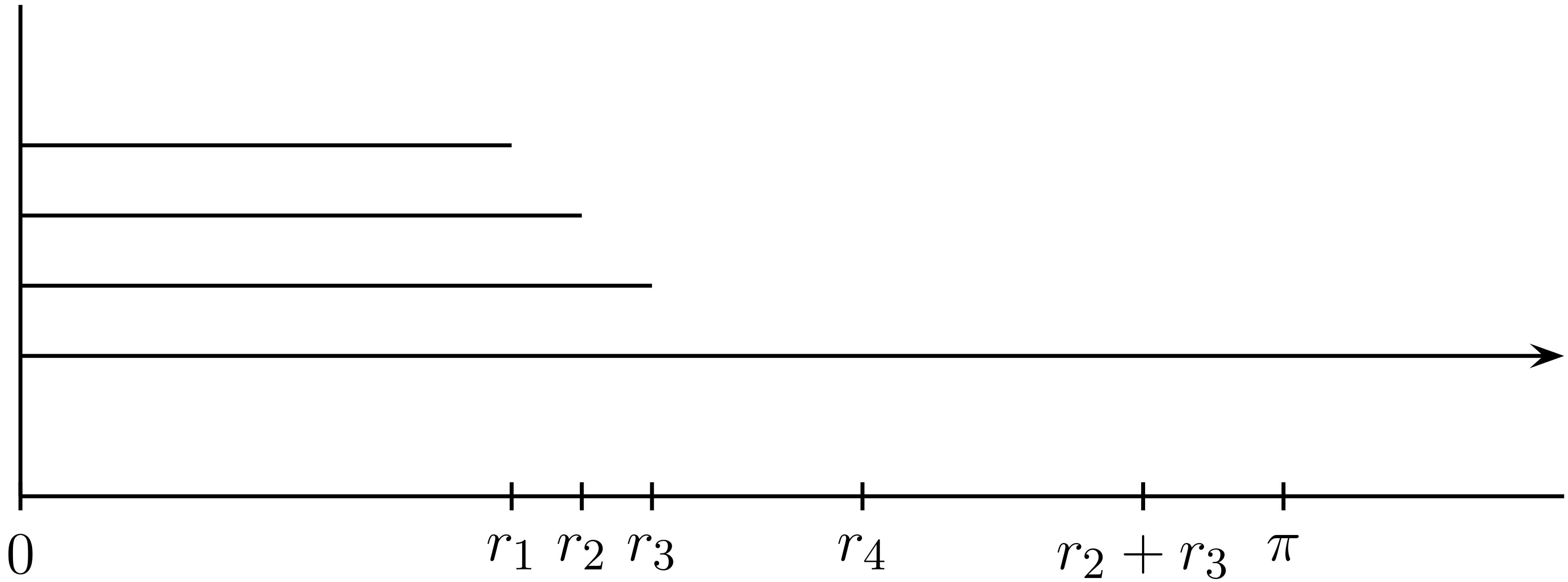


Betti 0-barcode



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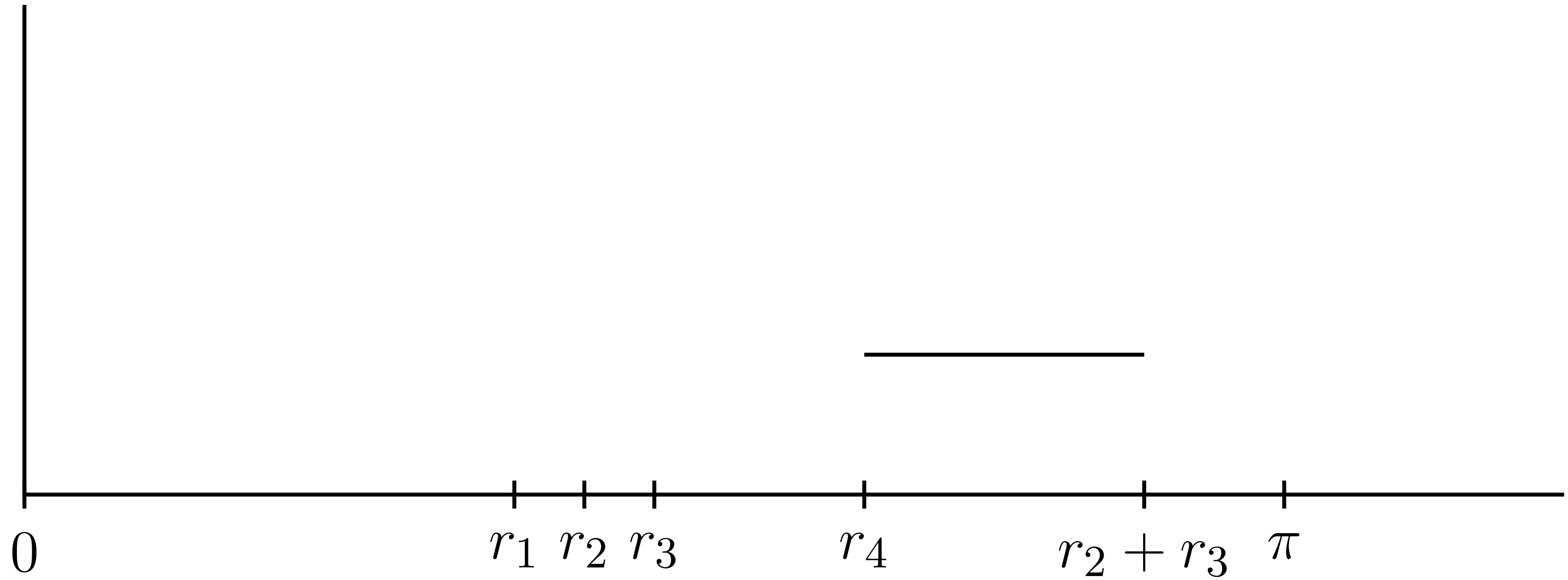

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5. Spacings

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For $2 \leq k \leq n$, choose $U_k \in [0, 1]$ such that

$$X_k = e^{2\pi i (\alpha + U_k)}.$$

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Order $\{U_2, \ldots U_n\}$ to obtain

$$0 < U_{n:1} < U_{n:2} < \ldots < U_{n:n-1} < 1.$$

Let $U_{n:0} = 0$ and $U_{n:n} = 1$.
For $1 \leq k \leq n$, let

$$S_k = U_{n:k} - U_{n:k-1}.$$

These are called the spacings.

Ordered Spacings

Order S:

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Let $B_0^n(k)$ equal the k-th shortest interval in the Betti-0 barcode.

Therefore,

$$B_0^n(k) = 2\pi S_{n:k}.$$

Uniform spacings

If X is sampled uniformly from S^1 then each U_k is uniform on $[0,1]$ and $S = (S_1, \ldots, S_n)$ are called uniform spacings.

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Assume X is sampled uniformly.

Lemma: $S = (S_1, \ldots, S_n)$ has a constant density on the standard $(n-1)$-simplex Δ^{n-1}

$$S_k \geq 0, \quad \sum_{k=1}^{n} S_i = 1.$$

Expected spacings

For $1 \leq k \leq n$, $ES_{n:k}$ can be found be integrating over Δ^{n-1}.

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Proposition:

$$ES_{n:k} = \frac{1}{n} \sum_{j=n+1-k}^{n} \frac{1}{j}$$

Corollary:

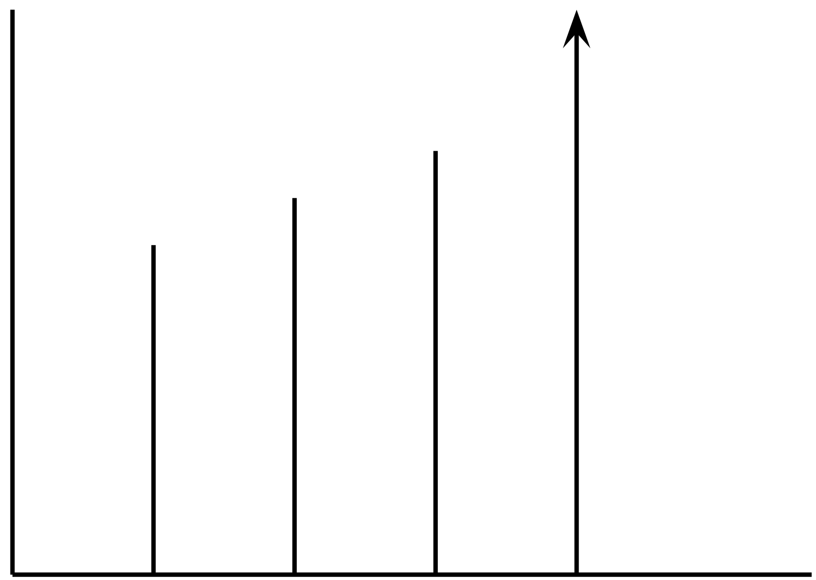
$$EB_0^n(k) = \frac{2\pi}{n} \sum_{j=n+1-k}^{n} \frac{1}{j}$$

6. Asymptotic behavior

We would like to understand what happens to the Betti barcodes as the number of samples n increases.

A different view

Consider the following view of the Betti-0 barcode.



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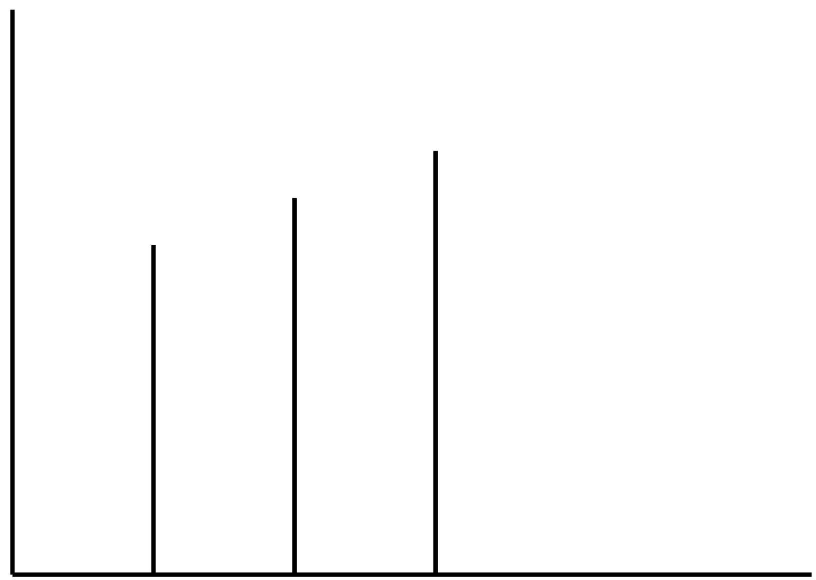

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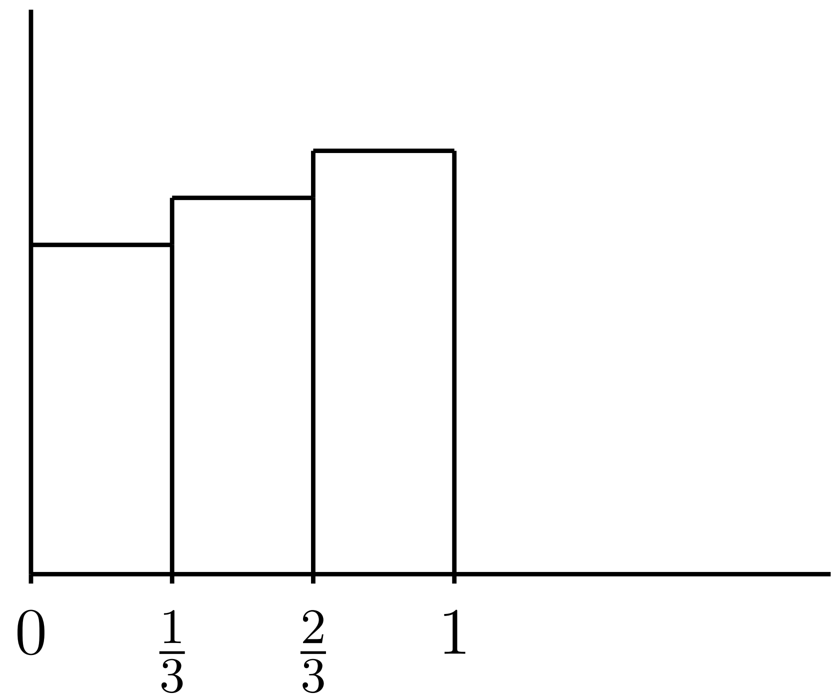

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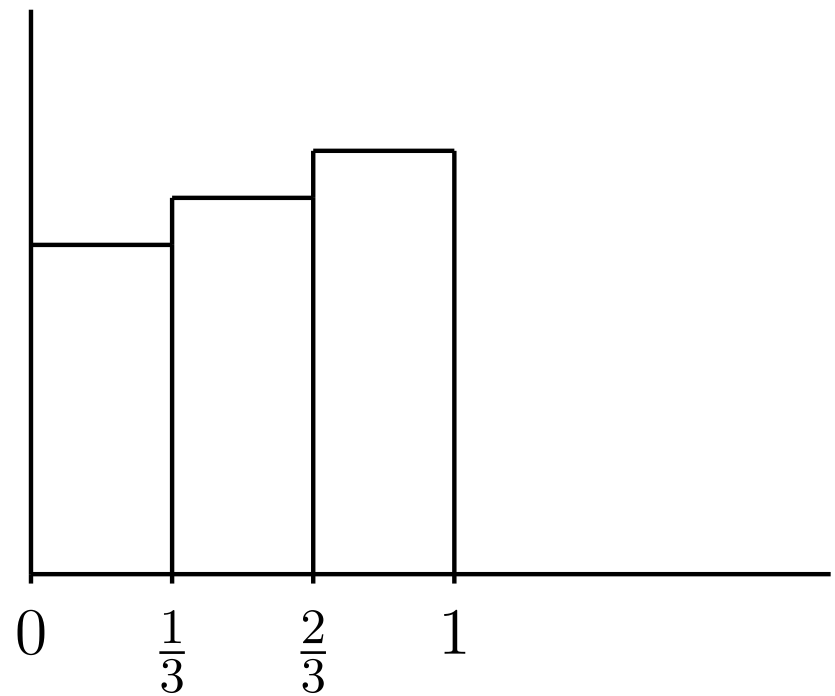

This gives us a function $B_0^n : [0,1] \longrightarrow \mathbf{R}_{\geq 0}$, where $B_0^n(x) = B_0^n(k)$, where $k = \lceil (n-1)x \rceil$.

Normalization

To see the effect of κ as $n \to \infty$, we normalize the above function.

$$\bar{B}_0^n(x) = \frac{B_0^n(x)}{\int_0^1 \; B_0^n(t)dt}$$

We call this the Betti-0 function.

Expected Betti-0 function

Recall that $B_0^n(x) = 2\pi S_{n:\lceil (n-1)x \rceil}$.

Thus,

$$\begin{aligned} E(B_0^n)(x) &= 2\pi E S_{n:\lceil (n-1)x \rceil} \\ &= \frac{2\pi}{n} \left(\sum_{j=n+1-\lceil (n-1)x \rceil}^{n} \frac{1}{j} \right). \end{aligned}$$

Expected Betti-0 function

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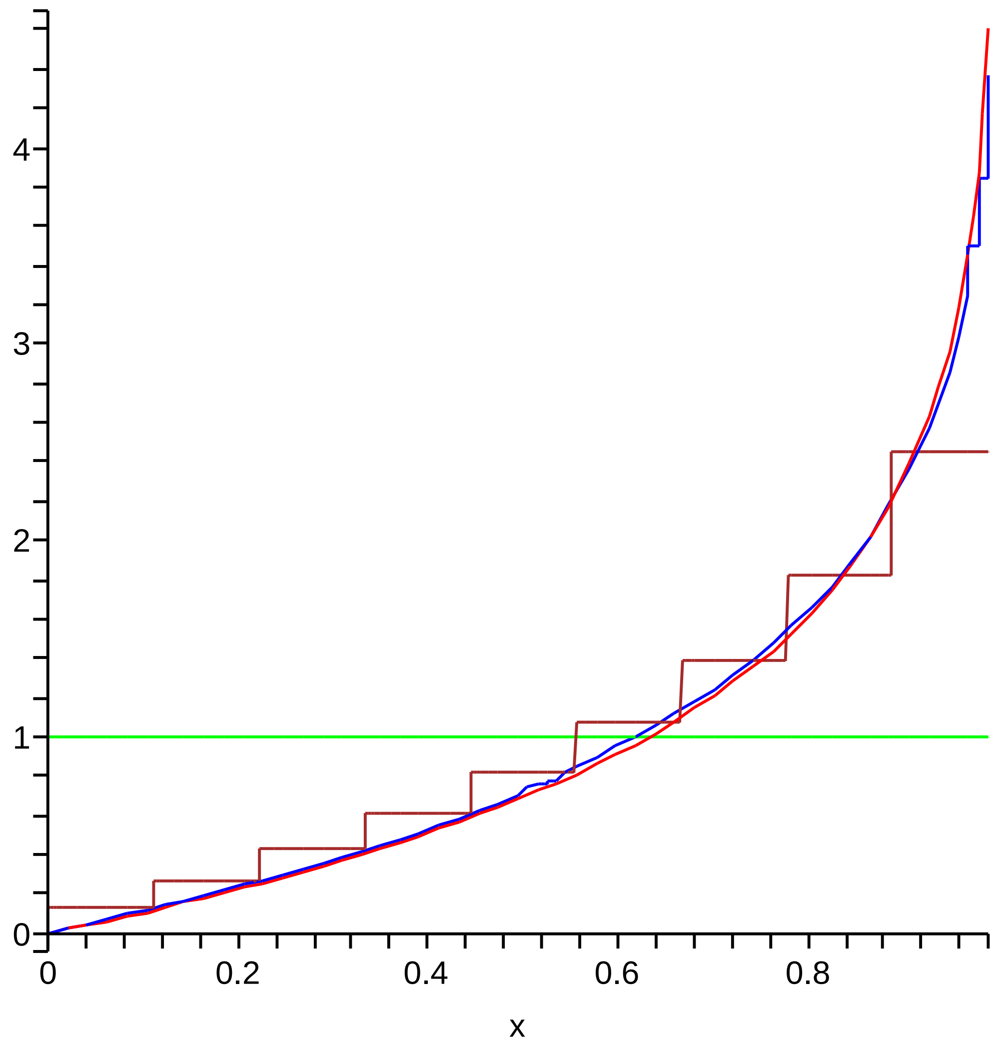
Proposition[B-K]:

$E(\bar{B}_0^n)(x) \to -\log(1-x)$ as $n \to \infty$.

Betti-0 Graphs



7. Topology of densities

We have also adapted persistent homology to study densities directly.

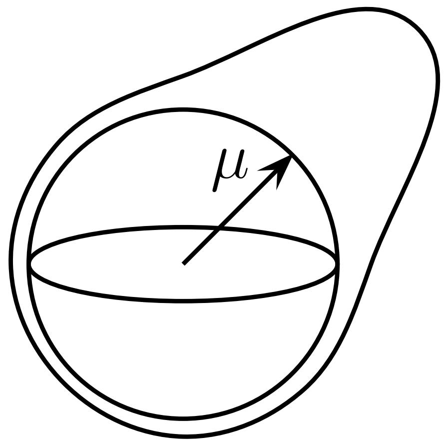
Recall that to use persistent homology one needs a parameter r.

We consider the portion of a manifold whose density is less that r, or alternately the portion whose density is greater than $\frac{1}{r}$.

Again we get Betti barcodes and Betti-0 functions.

The von Mises-Fischer distribution

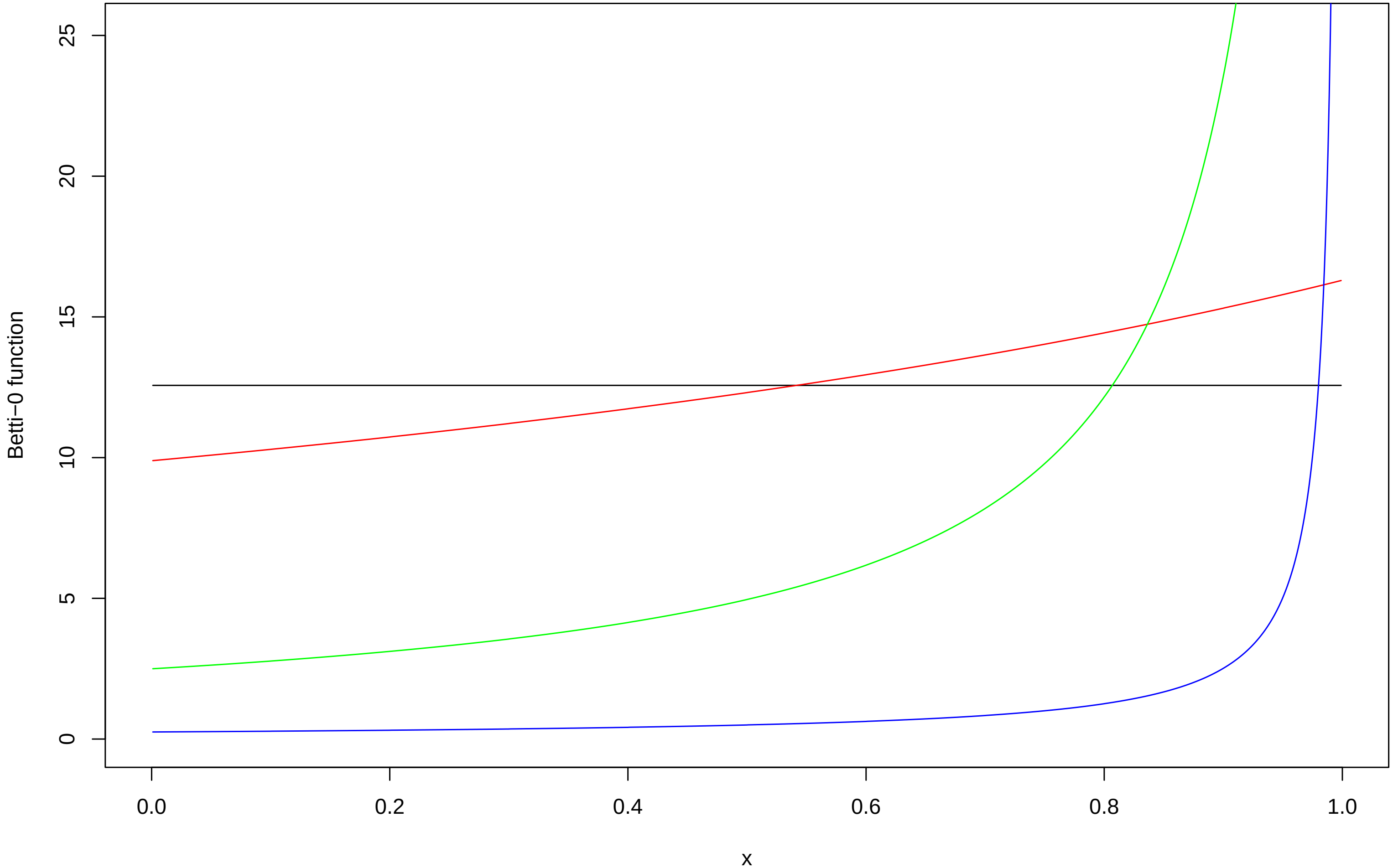
The von Mises-Fischer distribution gives unimodal density on S^{p-1}.



$$f_{\mu,\kappa}(x) = c(\kappa)e^{\kappa x^t \mu}.$$

For different values of κ we get different Betti barcodes and Betti-0 functions.

Betti-0 for various κ



The Betti-0 function for S^2 for $\kappa = 0, 0.25, 2.5, 25$

Maximum Likelihood Estimators

For PCD $x_1, \ldots, x_n$ on S^{p-1} sampled from the von Mises-Fischer distribution let $\bar{x}$ be the sample mean.

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A statistical estimator for μ is

$$\frac{\bar{x}}{\|\bar{x}\|}.$$

A statistical estimator for κ is

$$\hat{\kappa} = A_p^{-1}(\|\bar{x}\|) \text{ where } A_p(\lambda) = \frac{I_{p/2}(\lambda)}{I_{p/2-1}(\lambda)}.$$

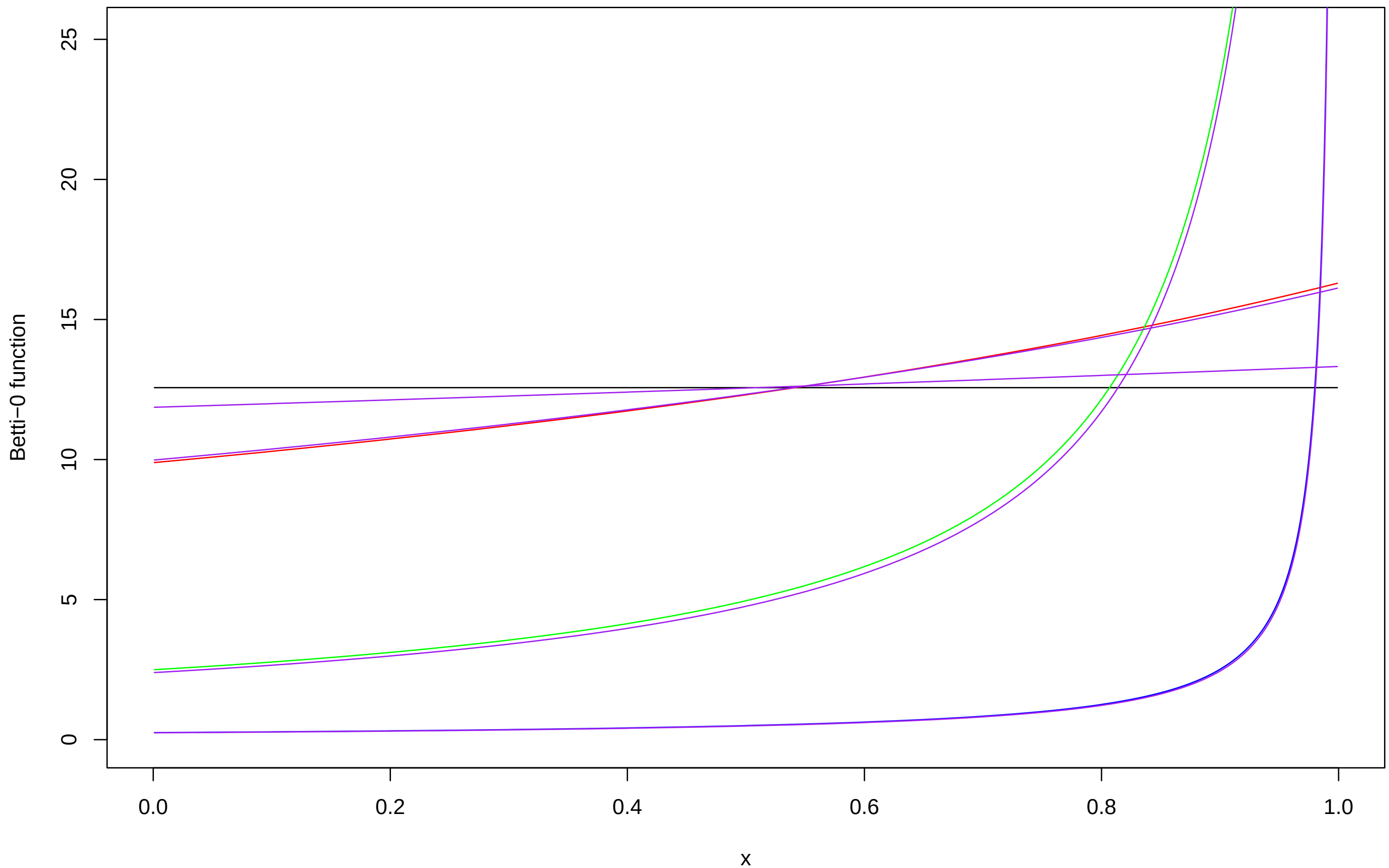
Example S^2

Simulating 1000 samples on S^2 from $\kappa = 0, 0.25, 2.5, 25$ we calculate the maximum likelihood estimators $\hat{\kappa}$.

We get $\hat{\kappa} = 0.058, 0.240, 2.611, 25.657$.

For these $\hat{\kappa}$, we can again calculate the Betti-0 functions.

Betti-0 for various $\kappa, \hat{\kappa}$



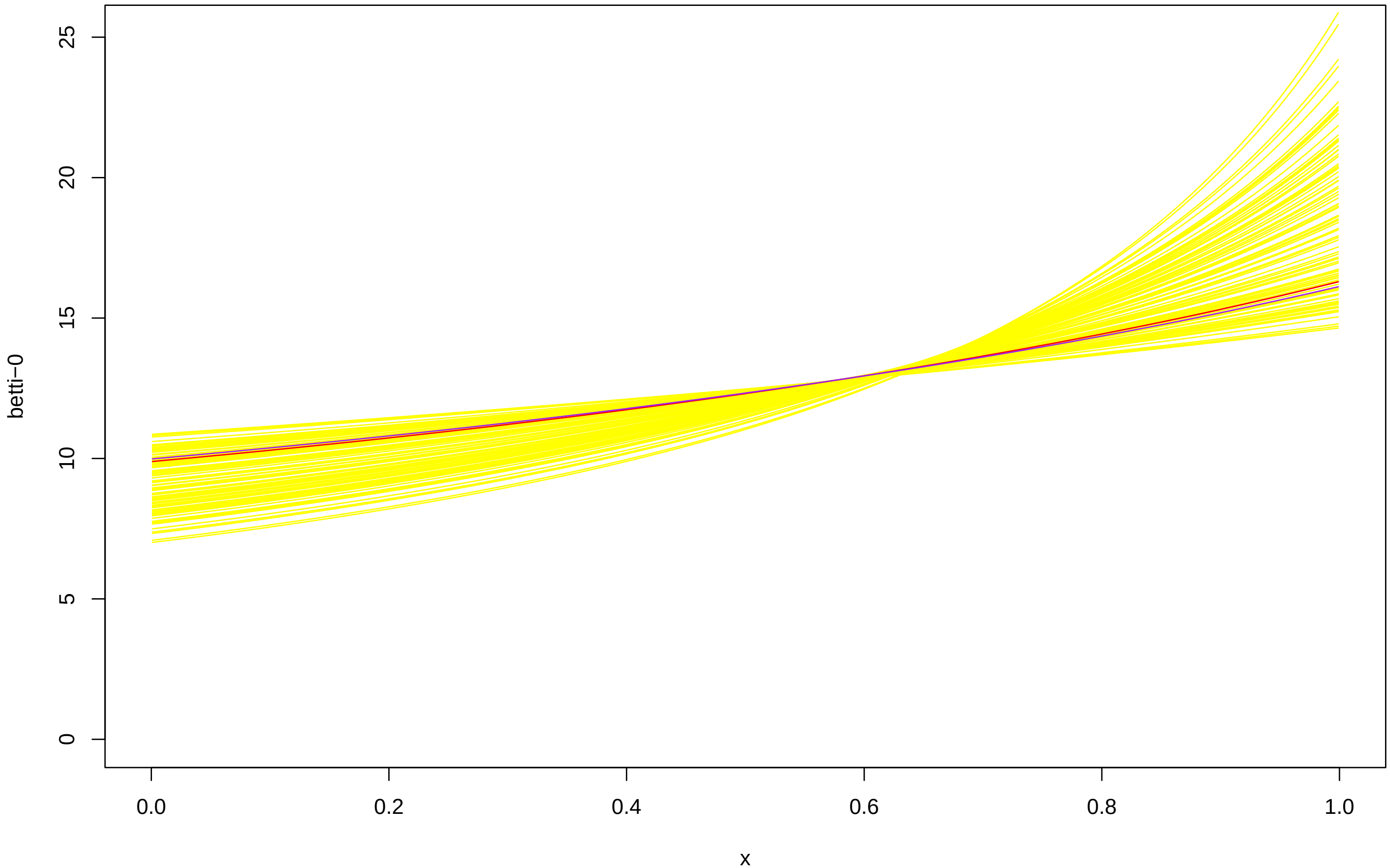
$$\kappa = 0, 0.25, 2.5, 25,\ \hat{\kappa} = 0.058, 0.240, 2.611, 25.657$$

Bootstrapping

Finally we sample from the maximum likelihood estimators, and again calculate the persistent homology.

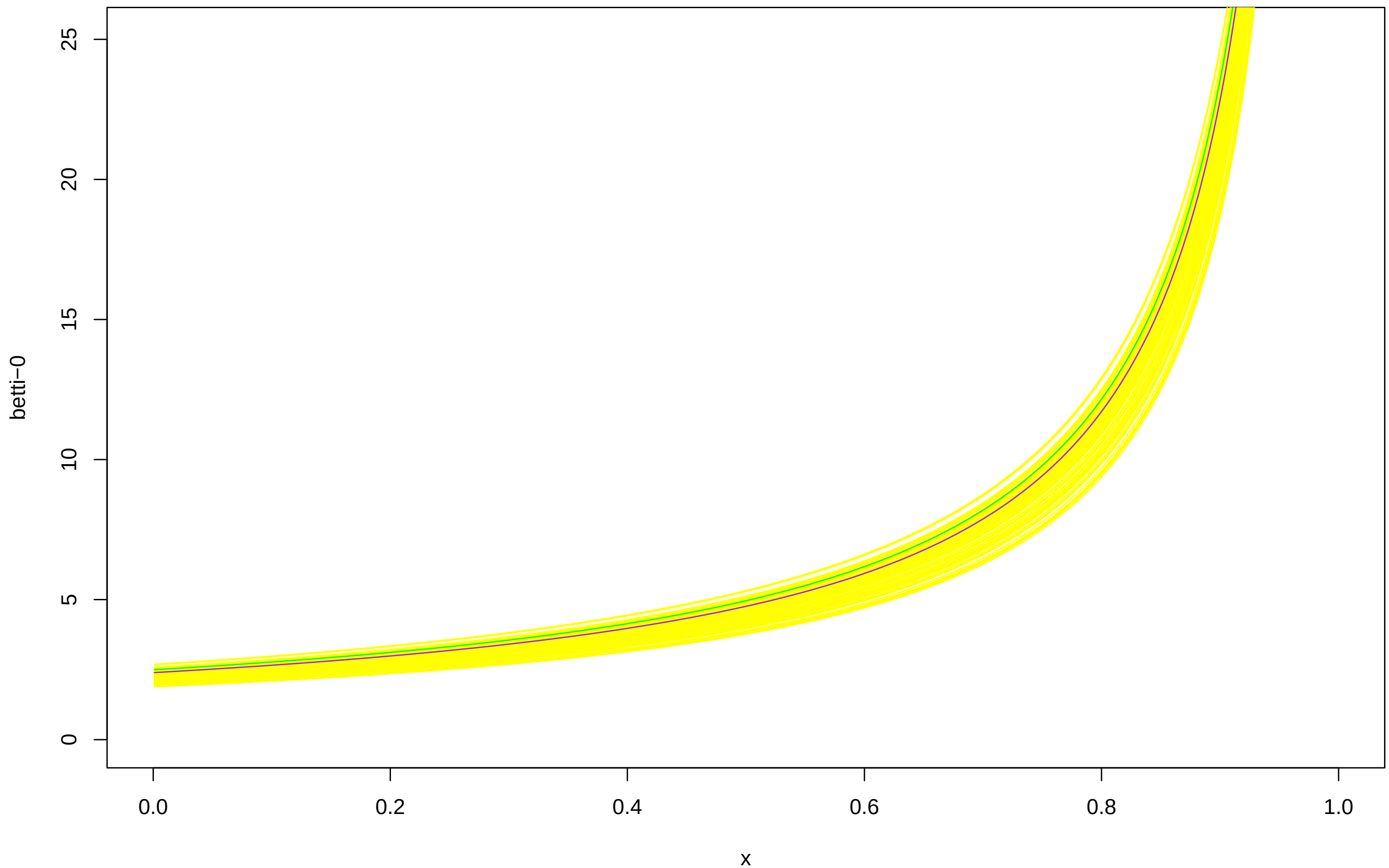
This provides confidence intervals on the Betti barcodes and Betti-0 functions.

Bootstrapping Betti-0



$\kappa = 0.25$, $\hat{\kappa} = 0.240$ and 95% bootstrap confidence interval

Bootstrapping Betti-0



$\kappa = 2.5$, $\hat{\kappa} = 2.611$ and 95% bootstrap confidence interval

Summary

- Persistent homology detects topological features of samples.
- Using the theory of spacings we were able to work out exact estimates of the Betti barcodes for samples on the uniform density on S^1.
- The asymptotic behaviour was $-\log(1-x)$.
- Applied directly to densities, persistent homology depends on the parameter.
- Using bootstrapping we can give confidence intervals on the Betti barcodes and the Betti-0 function of a sample.