Statistical Analysis of Persistent Homology

Genki Kusano (Tohoku University, D1)

Topology and Computer 2016, Oct 28 @ Akita.

Collaborators：

Kenji Fukumizu (The Institute of Statistical Mathematics）

Yasuaki Hiraoka (Tohoku University, AIMR)

Persistence weighted Gaussian kernel for topological data analysis.
Proceedings of the 33rd ICML, pp. 2004–2013, 2016

Self introduction

- Interests : Applied topology, topological data analysis

  B3 : Homology group, homological algebra

  B4 : Persistent homology, computational homology

  M1 : Applied topology to sensor network

  “**Relative interleavings and applications to sensor networks**”, JJIAM, 33(1),99-120, 2016.

  M2 : Statistics, machine learning, kernel methods

  “**Persistence weighted Gaussian kernel for topological data analysis**”, ICML, pp. 2004–2013, 2016.

  D1(now) : Time series analysis, dynamics, information geometry, …

- Announcement : Joint Mathematics Meetings, January 4, 2017, Atlanta

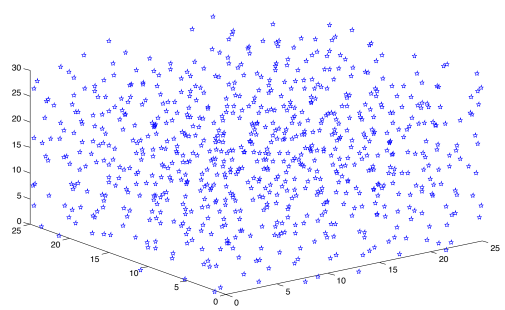
  ★Statistical Methods in Computational Topology and Applications

  Sheaves in Topological Data Analysis

Motivation of this work

Topological Data Analysis (TDA, 位相的データ解析)

Mathematical methods for characterizing “shapes of data”



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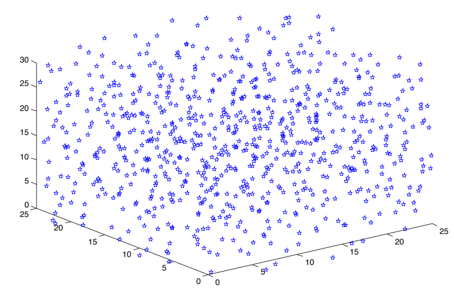
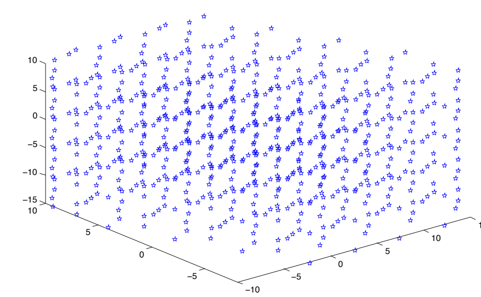




Liquid Glass Solid

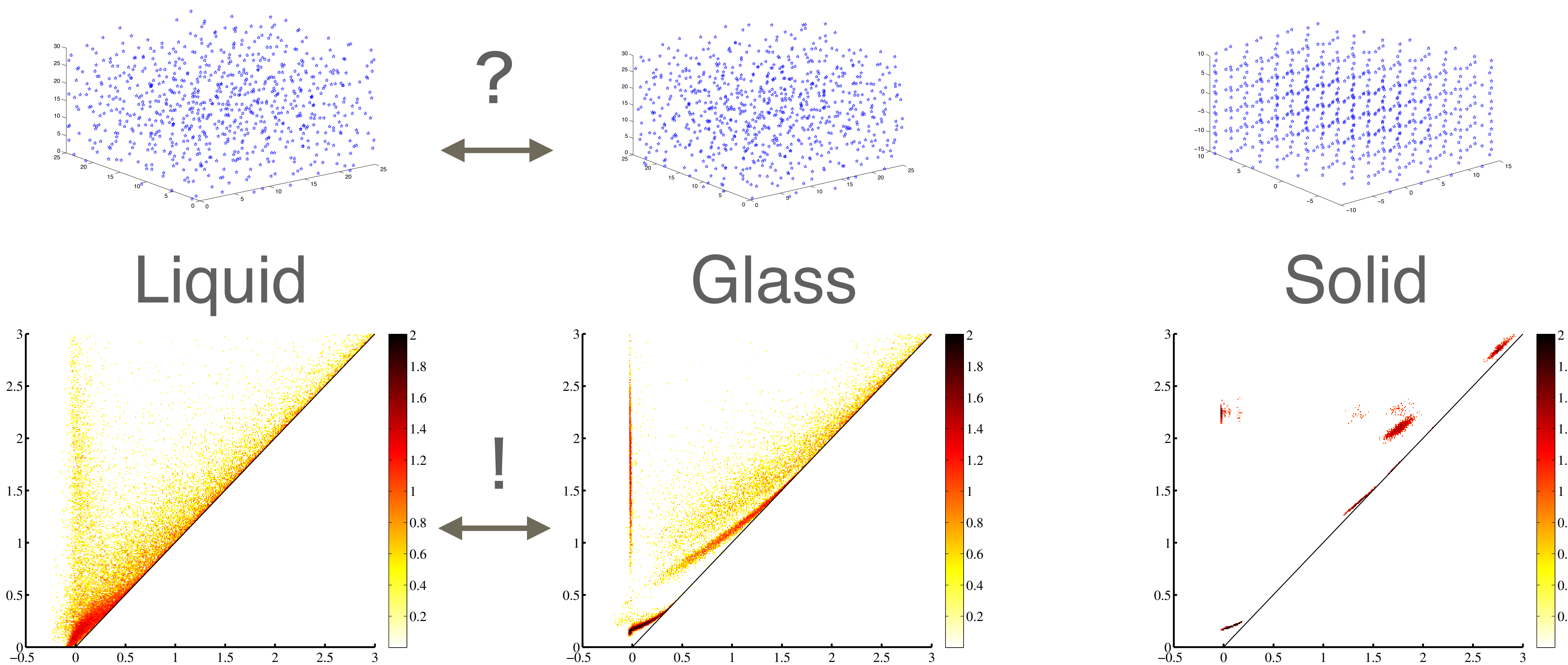
Atomic configurations of liquid, glass, and solid state of silica ($\mathrm{SiO_2}$, silica — composed of silicon and oxygen)

At the configuration level, it is difficult to distinguish liquid and glass state.

Motivation of this work

Persistent homology / Persistence diagram

Topological descriptor of data

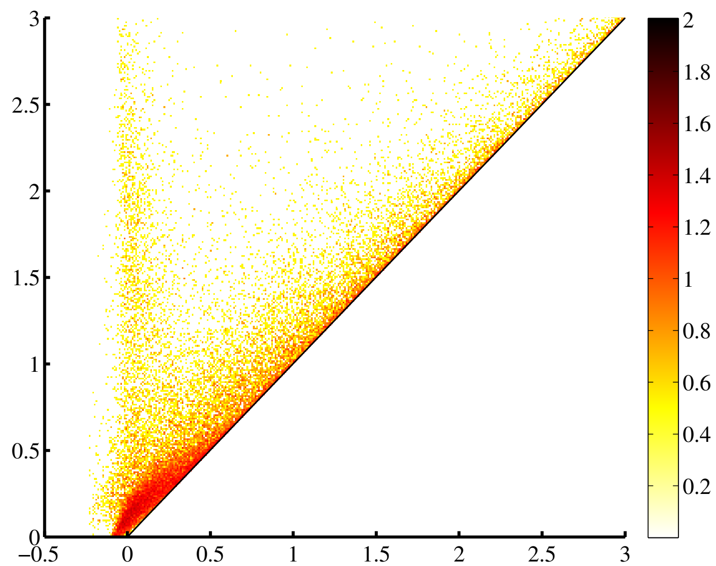


Y. Hiraoka et al., Hierarchical structures of amorphous solids characterized by persistent homology, PNAS, 113(26):7035–7040, 2016.

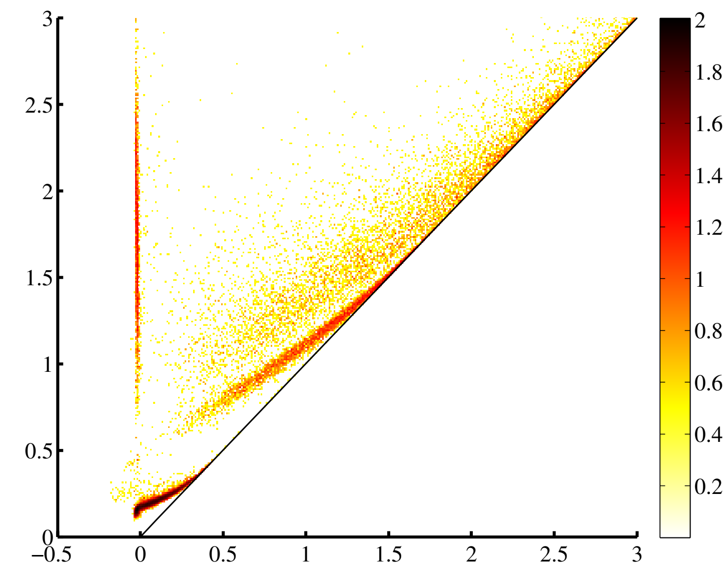
Motivation of this work

Classification problem

Liquid



Glass

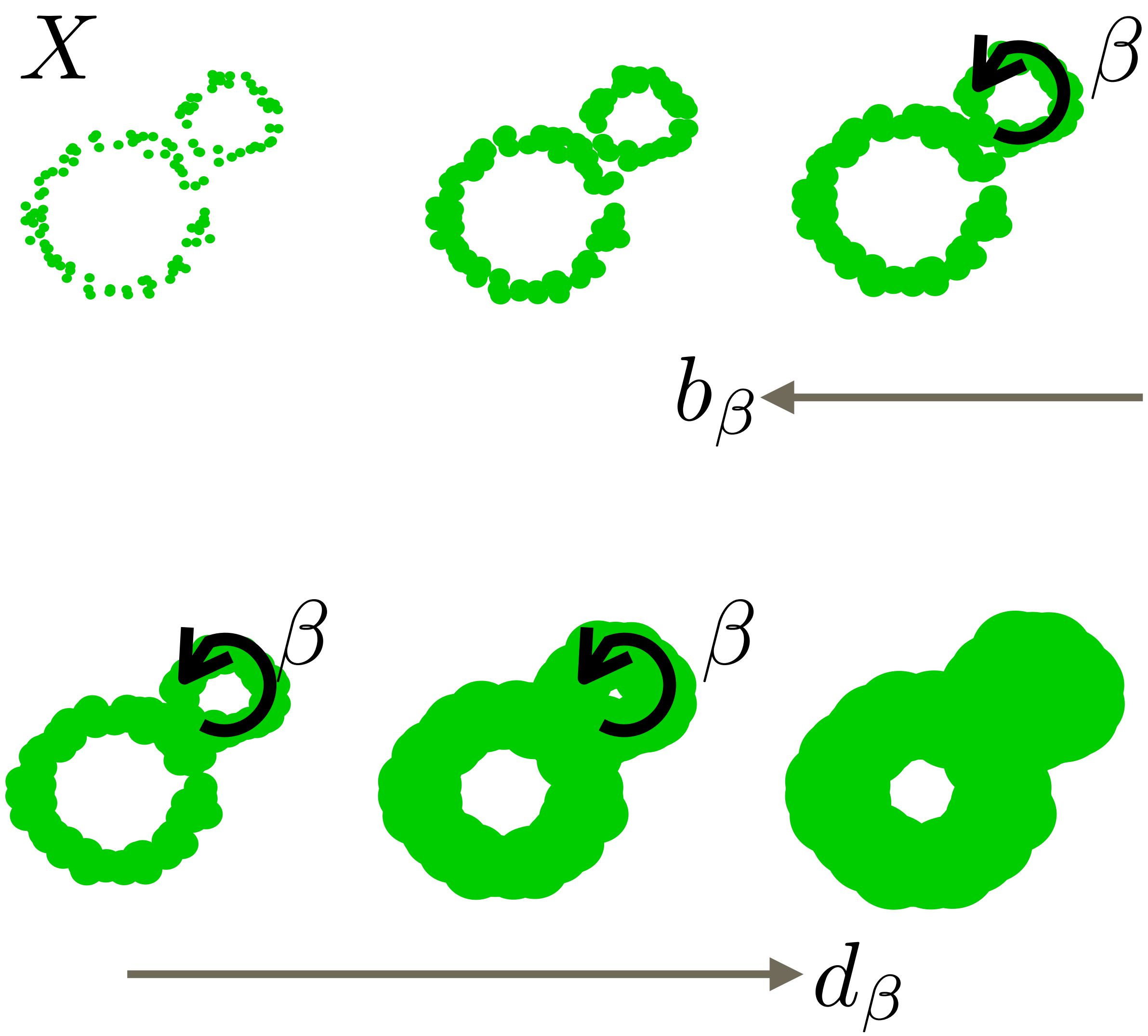


Q. Can we distinguish them mathematically?

A. Make a **statistical framework** for persistence diagrams

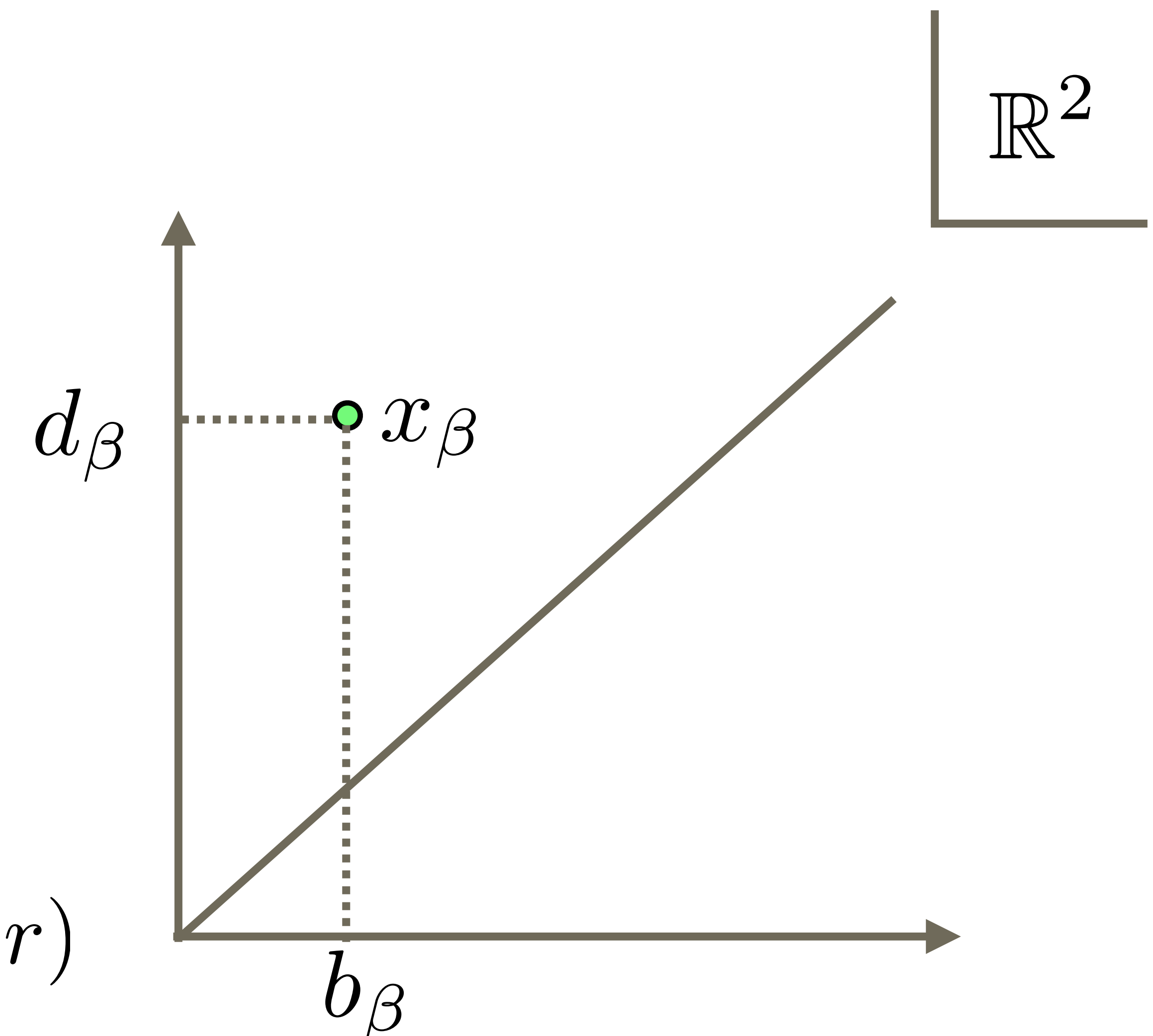
Section 1
What is a persistence diagram

Persistence diagram

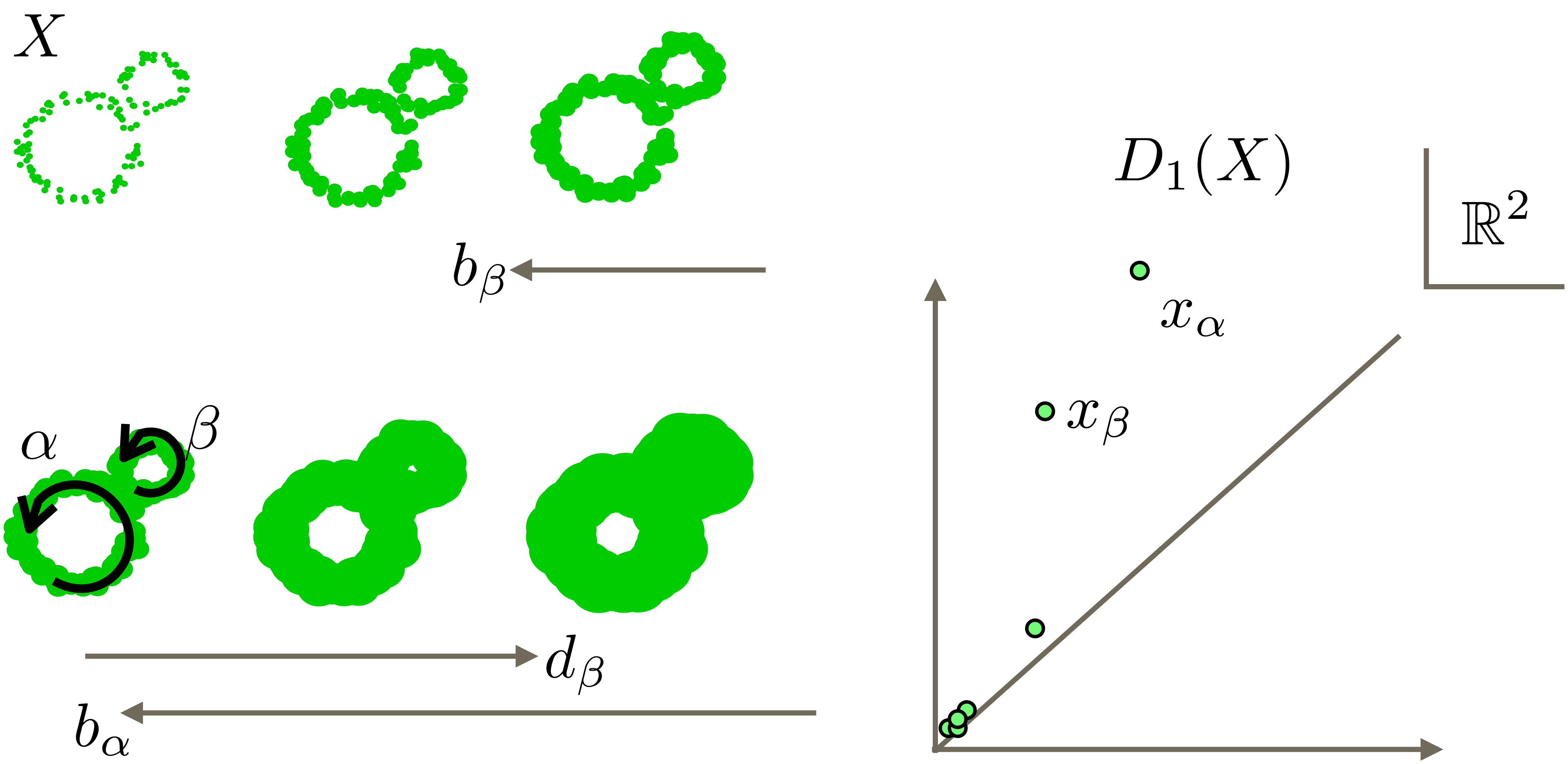


$$X_r = \bigcup_{x_i \in X} B(x_i; r)$$

$$B(x; r) = \{z \mid d(x,z) \le r\}$$



Persistence diagram



$$D_1(X) = \{x_\alpha, x_\beta, x_\gamma, \cdots \mid x_a = (b_\alpha, d_\alpha)\}$$

Definition of persistence diagram

Definition

For a filtration

$$\mathbb{X} : X_1 \subset X_2 \subset \cdots \subset X_n ,$$

we compute homology groups with a field coefficient K

and obtain a sequence

$$H_q(\mathbb{X}) : H_q(X_1) \to H_q(X_2) \to \cdots \to H_q(X_n) .$$

This sequence is called a persistent homology.

In this talk, we set a filtration by the union of balls

$$X_r = \bigcup_{x_i \in X} B(x_i; r)$$

A persistent homology $H_q(\mathbb{X})$ can be seen as a representation of $\mathbf{A}_n$ -quiver.

Definition of persistence diagram

From Gabriel and Krull-Remak-Schmidt theorem, there is the following decomposition:

$$H_q(\mathbb{X}) \cong \bigoplus_{i \in I} \mathbb{I}[b_i, d_i] \ (I \text{ is a finite set})$$

$$\mathbb{I}[b,d] : 0 \longleftrightarrow 0 \longleftrightarrow \cdots \longleftrightarrow 0 \longleftrightarrow \overset{b}{\mathbb{F}} \longleftrightarrow \mathbb{F} \longleftrightarrow \cdots \longleftrightarrow \overset{d}{\mathbb{F}} \longleftrightarrow 0 \longleftrightarrow \cdots \longleftrightarrow 0$$

From the decomposition $H_q(\mathbb{X}) \cong \bigoplus_{i \in I} \mathbb{I}[b_i, d_i]$,

the persistence diagram is defined by $D_q(\mathbb{X}) = \{(b_i, d_i) \mid i \in I\}$.

Remark: $\bigoplus_r H_q(X_r)$ can be seen as a module over $K[t]$ and it can be decomposed from the structure theorem for PID.

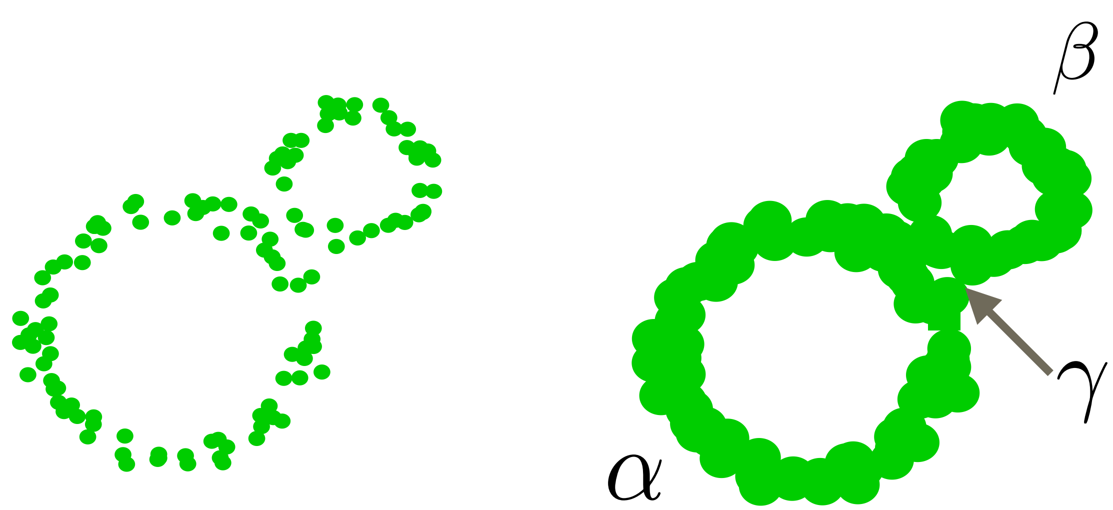
Persistence

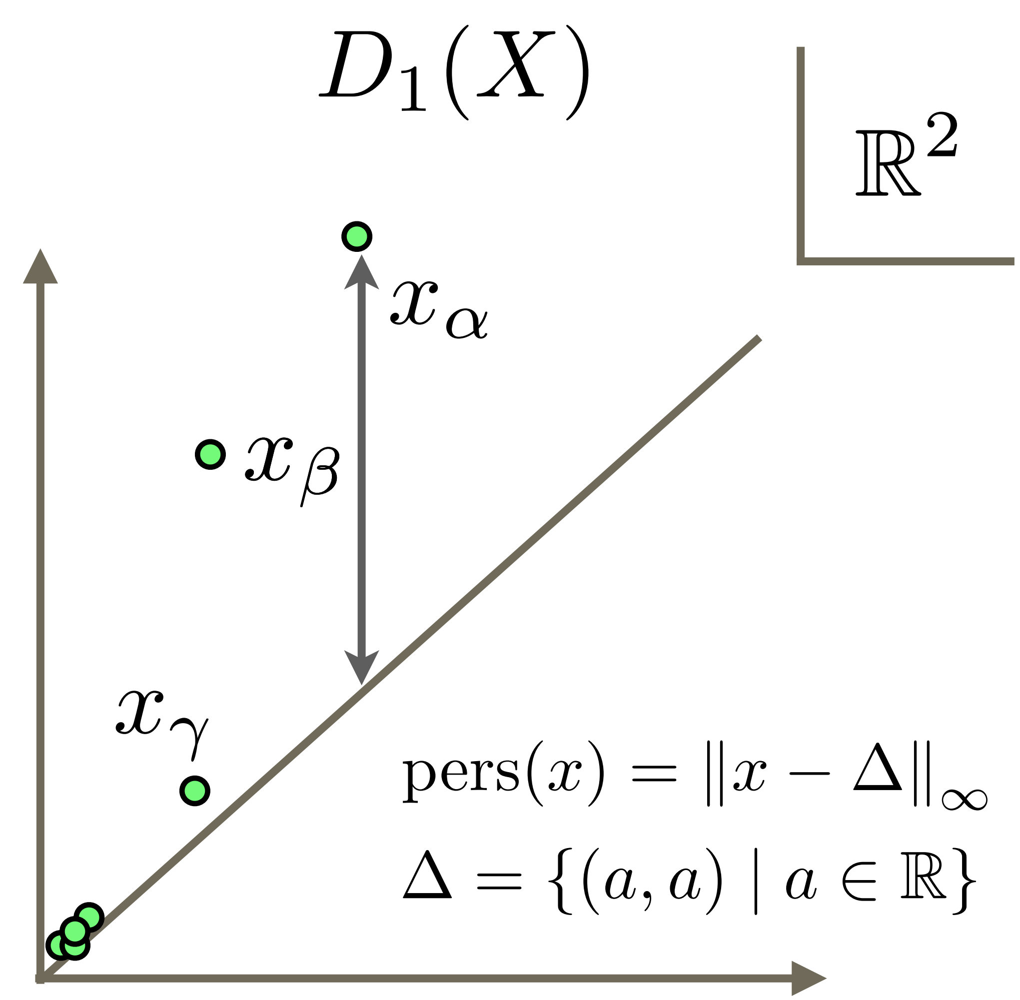
Definition

The lifetime of a cycle x_α

$$\mathrm{pers}(x_\alpha) = d_\alpha - b_\alpha$$

is called persistence.





A cycle with small persistence can be seen as a small cycle, and sometimes noisy cycle.

Metric structure of persistence diagram

The set of persistence diagrams is defined by

$$\mathcal{D} = \{D \mid D \text{ is a multiset in } \mathbb{R}^2_{ul} \text{ and } |D| < \infty\},$$

where $\mathbb{R}^2_{ul} = \{(b,d) \mid b \leq d \in \mathbb{R}\}$.

The **bottleneck (∞-Wasserstein) metric**

$$d_B(D,E) = \inf_{\gamma} \sup_{x \in D \cup \Delta} \|x - \gamma(x)\|_\infty \ (\gamma : D \cup \Delta \to E \cup \Delta \text{ is bijective}),$$

where $\Delta = \{(a,a) \mid a \in \mathbb{R}\}$ is the diagonal set,
becomes a distance on the set of persistence diagrams.

Remark: $(\mathcal{D}, d_B)$ is a metric space.

Stability theorem

Theorem[Cohen-Steiner et al., 2007]

For finite subsets $X, Y \subset \mathbb{R}^d$, $d_B(D_q(X), D_q(Y)) \leq d_H(X, Y)$,

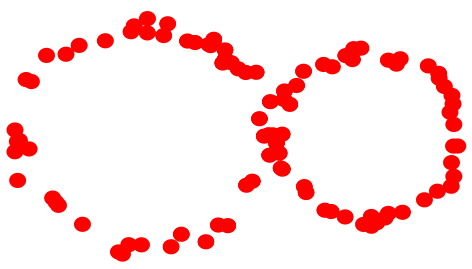
where $d_H(X,Y) = \max\left\{\max_{p\in X}\min_{q\in Y} d(p,q), \max_{q\in Y}\min_{p\in X} d(p,q)\right\}$ is the Hausdorff distance.

Significant property

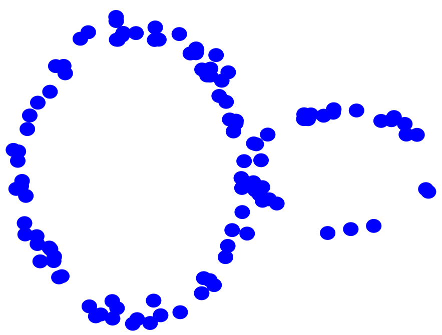
This map $X \rightarrow D_q(X)$ is Lipchitz continuous.

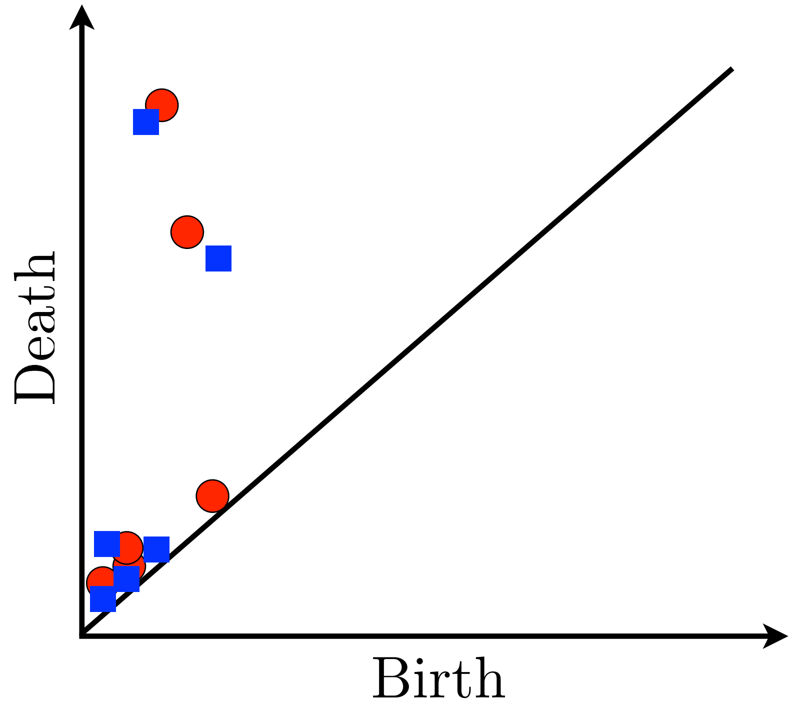
(Betti number $X \rightarrow \beta_q(X) = \dim H_q(X)$ is not continuous.)

X



Y





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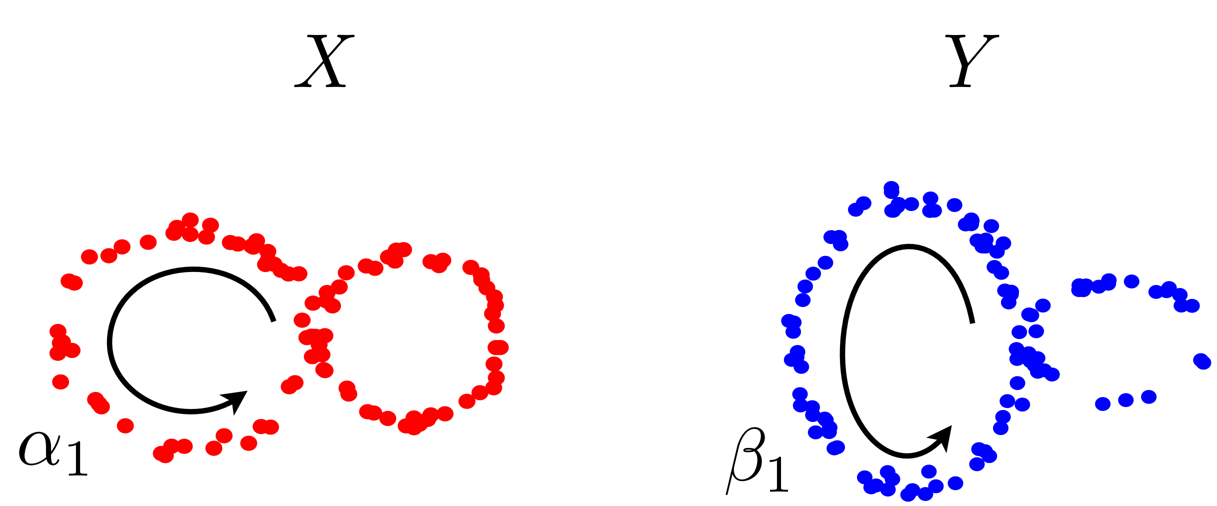
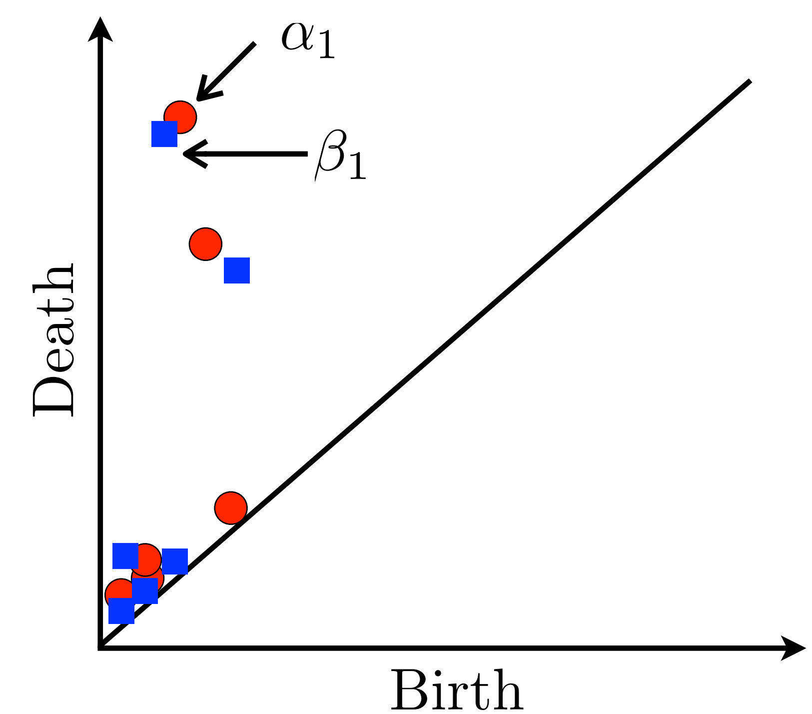




Statistical Topological Data Analysis

Data → Persistence diagram → Prediction / Classification / Testing / Estimation

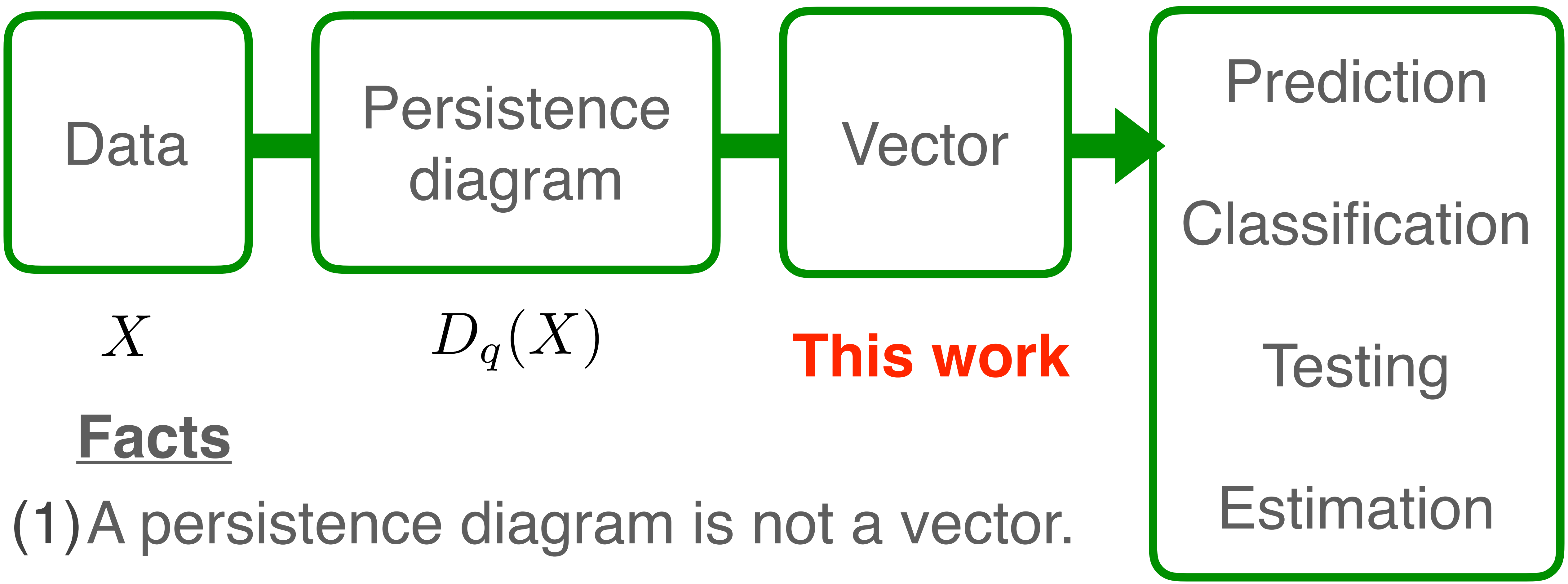
X $D_q(X)$

Facts

(1) A persistence diagram is not a vector.

(2) Standard statistical method is for vectors (multivariate analysis)

Statistical Topological Data Analysis



Facts

(1) A persistence diagram is not a vector.

(2) Standard statistical method is for vectors (multivariate analysis)

Make a vector representation of persistence diagram by kernel method

Section 2
Kernel method
~Statistical method for non-vector data~

Statistics for non-vector data

Let Ω be a data set and $x_1, \cdots, x_n \in \Omega$ be obtained data.

To consider statistical properties of the data, it is sometimes needed to calculate summaries, like mean/average:

$$x_1, \cdots, x_n \to \frac{1}{n}\sum_{i=1}^{n} x_i$$

To calculate statistical summaries, the data set Ω is desired to have structures of addition, multiplication by scalers, and inner product, that is, Ω should be an inner product space.

The space of persistence diagrams is not an inner space.

Statistics for non-vector data

While Ω does not always have an inner product, by defining a map $\phi : \Omega \to H$, where H is an inner product space, we can consider statistical summaries in H.

$$x_1, \cdots, x_n \to \phi(x_1), \cdots, \phi(x_n) \to \frac{1}{n}\sum_{i=1}^{n} \phi(x_i) \in H$$

(well-defined)

<u>Fact</u>

Many statistical summaries and machine learning techniques are calculated from the value of inner product:

$$\langle \phi(x_i), \phi(x_j) \rangle_H$$

Kernel method

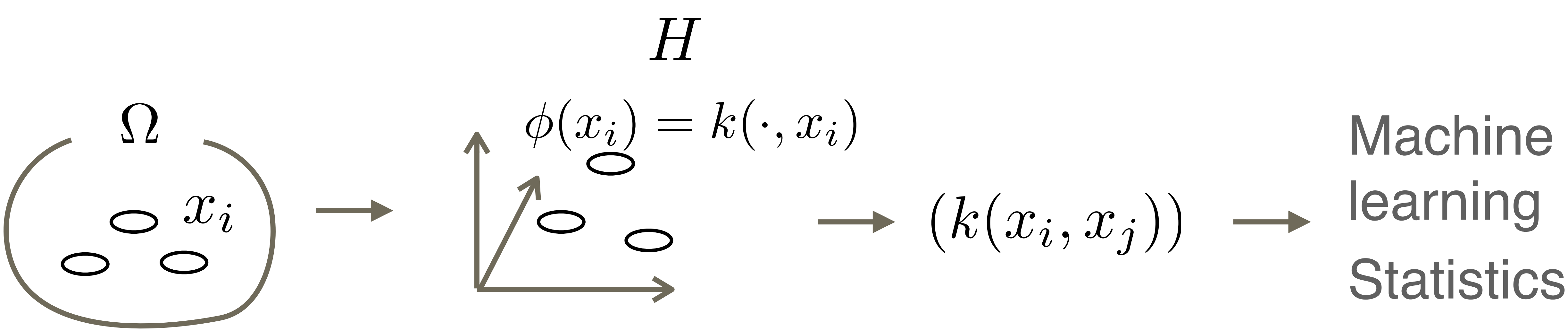
In kernel method, a positive definite kernel $k : \Omega \times \Omega \to \mathbb{R}$ is used as "non-linear" inner product on the data set.

$$k(x, y) = \langle \phi(x), \phi(y) \rangle_H$$

For an element $x \in \Omega$, $k(\cdot, x) : \Omega \to \mathbb{R}$ is a function and a vector in the functional space $C(\Omega)$.

In many cases, what we need is just the Gram matrix

$$(k(x_i, x_j))_{i,j=1,\cdots,n}$$



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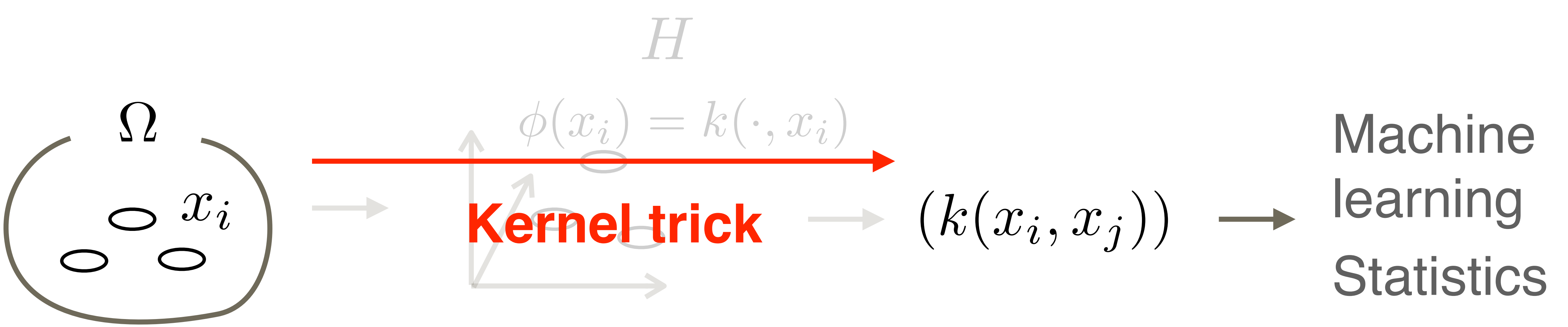


Kernel method

Definition

Let Ω be a set. A function $k : \Omega \times \Omega \to \mathbb{R}$ is called a positive definite kernel when k satisfies

- $k(x, y) = k(y, x)$
- For any $x_1, \ldots, x_n \in \Omega$, the matrix $(k(x_i, x_j))$ is semi-positive definite (this matrix is called the Gram matrix).

Examples in case of $\Omega = \mathbb{R}^d$,

- linear kernel $k_L(x, y) = \langle x, y \rangle$
- polynominal kernel $k_P(x, y) = (\langle x, y \rangle + c)^d$
- **Gaussian kernel** $k_G(x, y) = e^{-\frac{\|x-y\|^2}{2\sigma^2}}$

Kernel method

Moore-Aronszajn theorem

A p.d. kernel k uniquely defines a Hilbert space $\mathcal{H}_k$ which is called reproducing kernel Hilbert space (RKHS) satisfying

- for any $x \in \Omega$, the function $k(\cdot, x) : \Omega \to \mathbb{R}$ is in $\mathcal{H}_k$.
- $\mathrm{Span}\{k(\cdot, x) \mid x \in \Omega\}$ is dense in $\mathcal{H}_k$.
- for any $x \in \Omega$ and $f \in \mathcal{H}_k$, $\langle f, k(\cdot, x)\rangle_{\mathcal{H}_k} = f(x)$.

That is, $k(\cdot, x) : \Omega \to \mathbb{R}$ is an element of the Hilbert space $\mathcal{H}_k$.
(**RKHS vector**)

The inner product is computed by

$$\langle k(\cdot, y), k(\cdot, x)\rangle_{\mathcal{H}_k} = k(x, y)\ .$$

Kernel embedding

In order to consider statistical properties of (probability) distributions on Ω, we vectorize them by a positive definite kernel.

Here, let Ω be a locally compact Hausdorff space and $M_b(\Omega)$ be the set of finite signed Radon measures. Then, measures can be represented as an element of RKHS:

$$M_b(\Omega) \ni \mu \mapsto E_k(\mu) := \int k(\cdot, x) d\mu(x) \in \mathcal{H}_k$$

This map is called kernel embedding and this integral is interpreted as the Bochner integral.

Kernel embedding

If a kernel is "nice", the kernel embedding becomes injective.

$$M_b(\Omega) \ni \mu \mapsto E_k(\mu) := \int k(\cdot, x) d\mu(x) \in \mathcal{H}_k$$

The Gaussian kernel $k_G(x, y) = e^{-\frac{\|x-y\|^2}{2\sigma^2}}$ is C_0-universal.

Definition

A p.d. kernel k is said to be C_0**-universal** if $k(\cdot, x)$ is in $C_0(\Omega)$ and $\mathcal{H}_k$ is dense in $C_0(\Omega)$.

Proposition [B.K. Sriperumbudur et al., 2011]

If k is C_0-universal, E_k is injective, and hence

$d_k(\mu, \nu) := \|E_k(\mu) - E_k(\nu)\|_{\mathcal{H}_k}$ becomes a metric on $M_b(\Omega)$.

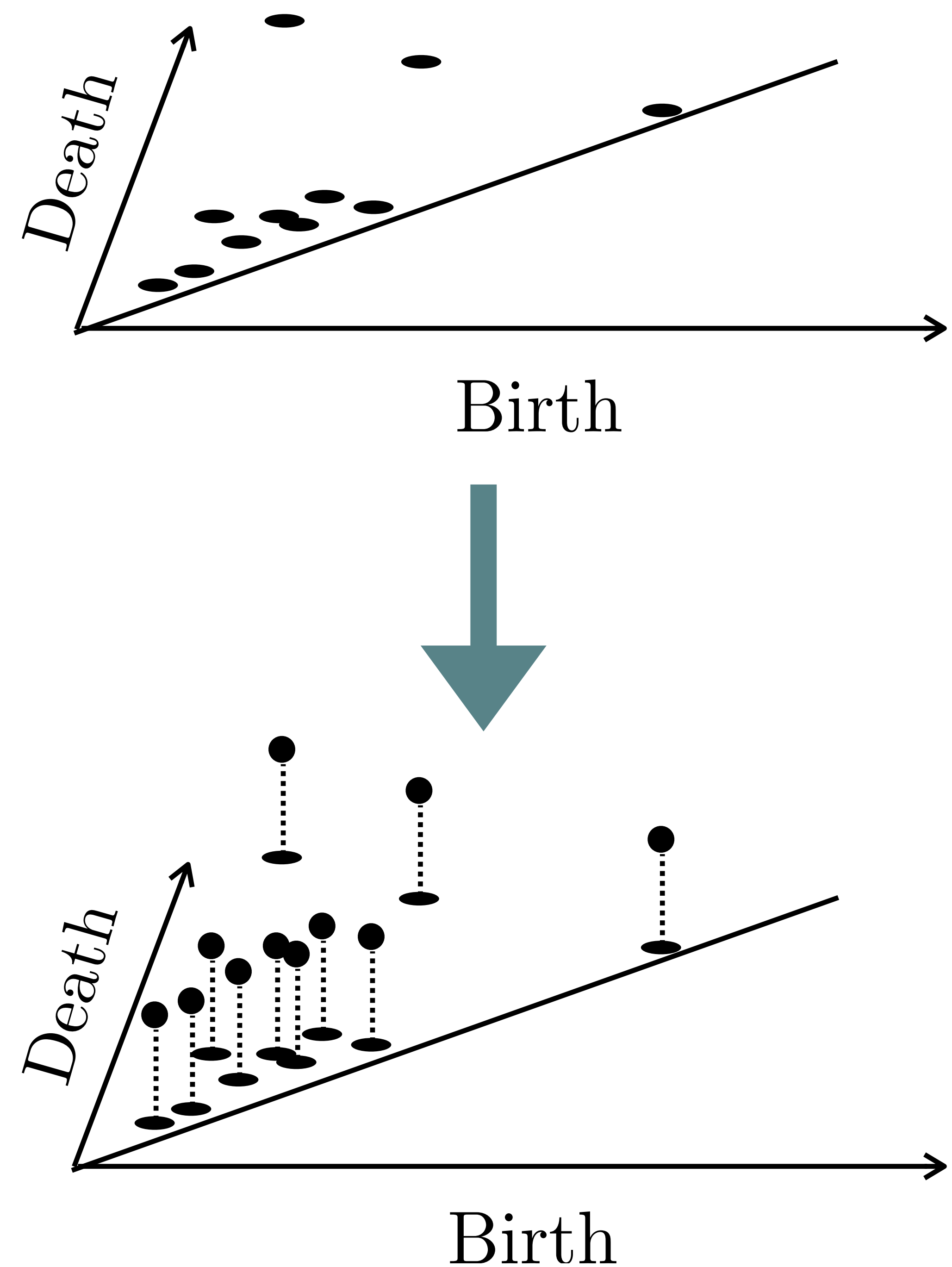
Section 3
Kernel on persistence diagram

Kernel on persistence diagram

A persistence diagram can be seen as a counting measure

$$\mu_D = \sum_{x \in D} \delta_x$$

where δ_x is the Delta measure.



<u>Observation</u>
Point close to the diagonal has a small persistence, so it sometimes can be seen as a noisy cycle.

Kernel on persistence diagram

A persistence diagram can be seen as a counting measure

$$\mu_D = \sum_{x \in D} \delta_x$$

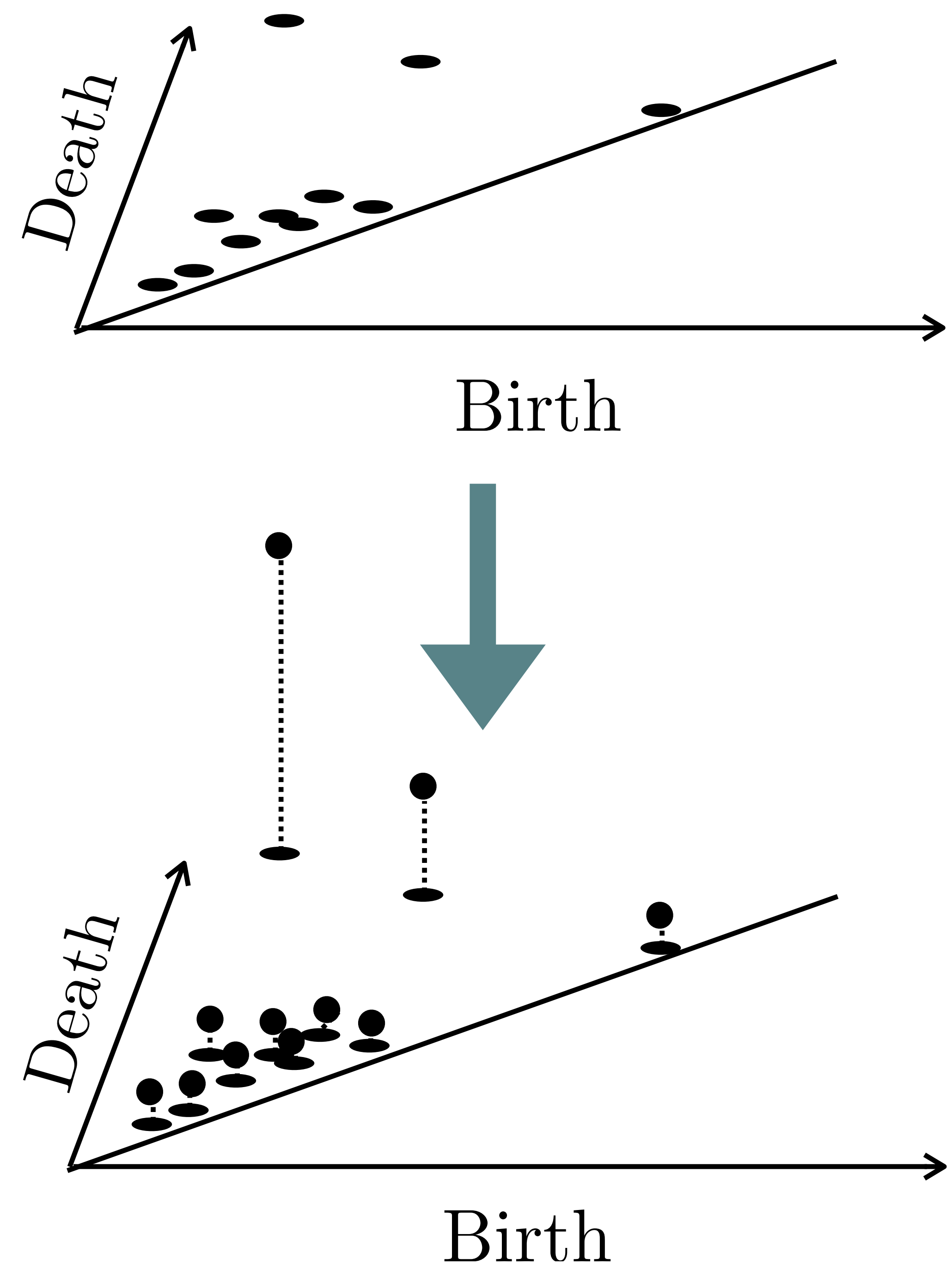
where δ_x is the Delta measure.

By defining an appropriate function

$$w : \mathbb{R}^2 \to \mathbb{R} \ ,$$

a persistence diagram is represented as a **weighted** measure:

$$\mu_D^w = \sum_{x \in D} w(x)\delta_x$$



Kernel on persistence diagram

For the weighted measure, we consider the kernel embedding:

$$D \mapsto \mu_D^w \mapsto E_k(\mu_D^w) = \sum_{x \in D} w(x) k(\cdot, x) \in \mathcal{H}_k$$

Then, we define a kernel on persistence diagram as the Gaussian kernel on the RKHS:

$$K_G(D, E) = \exp\left(-\frac{1}{2\tau^2} \left\| E_k(\mu_D^w) - E_k(\mu_E^w) \right\|_{\mathcal{H}_k}^2 \right)$$

We can define a linear kernel on RKHS

$$K_L(D, E) = \langle E_k(\mu_D^w), E_k(\mu_E^w) \rangle_{\mathcal{H}_k}$$

Metric on RKHS vectors

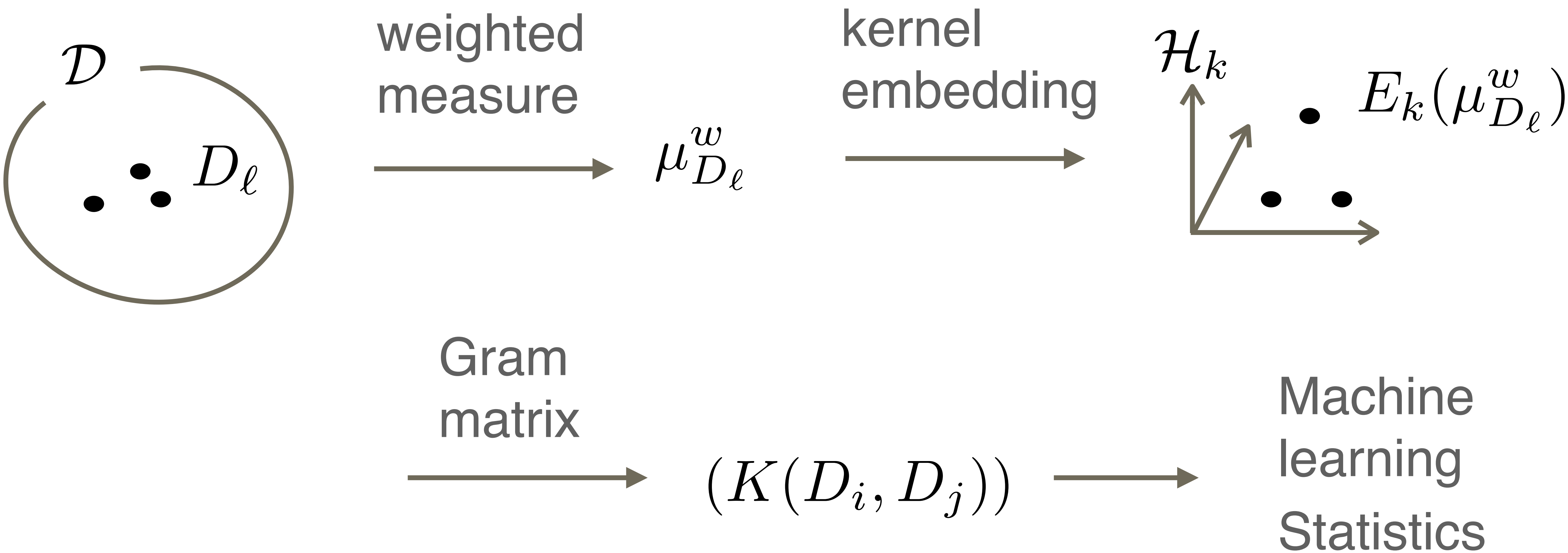
While the vector $E_k(\mu_D^w)$ is an element of $\mathcal{H}_k \subset C(\mathbb{R}^2_{ul})$, the inner product is easy to compute:

$$\langle E_k(\mu_D^w), E_k(\mu_E^w)\rangle_{\mathcal{H}_k} = \sum_{x\in D}\sum_{y\in E} w(x)w(y)k(x,y)\,.$$

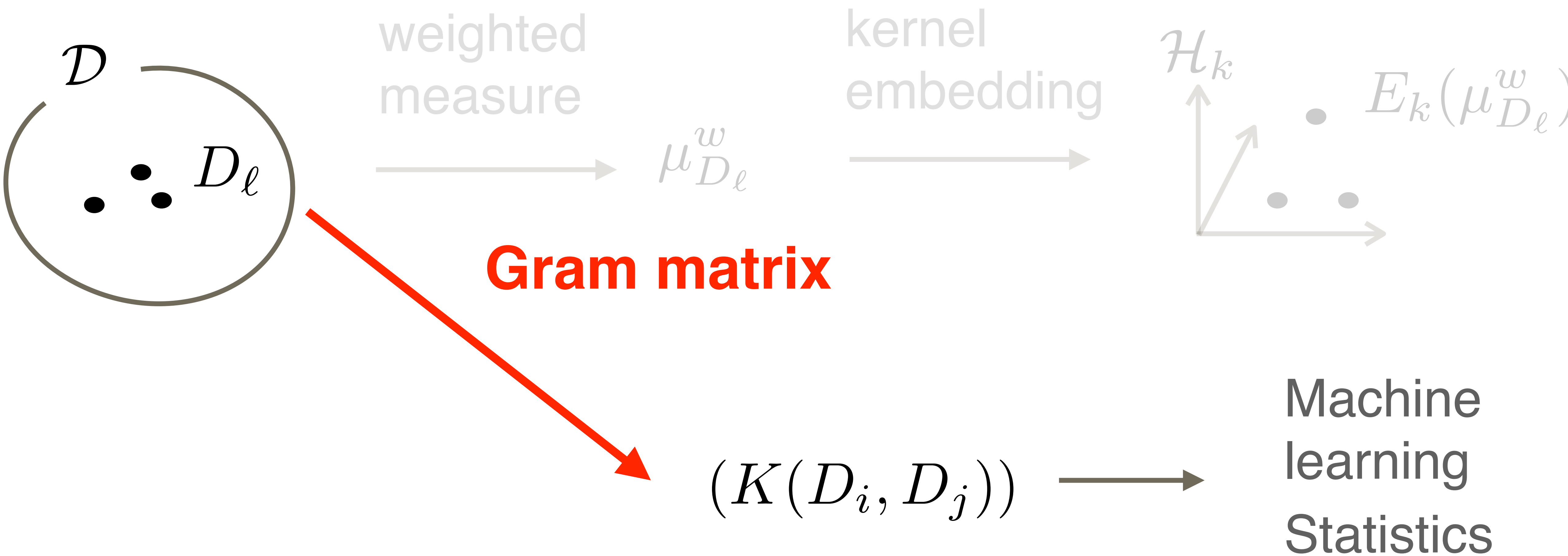
The distance also has the following expansion:

$$\begin{aligned}\|E_k(\mu_D^w) - E_k(\mu_E^w)\|^2_{\mathcal{H}_k} = &\sum_{x\in D}\sum_{x'\in D} w(x)w(x')k(x,x') + \sum_{y\in E}\sum_{y'\in E} w(y)w(y')k(y,y') \\ &- 2\sum_{x\in D}\sum_{y\in E} w(x)w(y)k(x,y)\end{aligned}$$

Kernel on persistence diagram



Kernel on persistence diagram



$$K_G(D,E) = \exp\left(-\frac{1}{2\tau^2}\|E_k(\mu^w_D) - E_k(\mu^w_E)\|^2_{\mathcal{H}_k}\right)$$

$$\|E_k(\mu^w_D) - E_k(\mu^w_E)\|^2_{\mathcal{H}_k} = \sum_{x\in D}\sum_{x'\in D} w(x)w(x')k(x,x') + \sum_{y\in E}\sum_{y'\in E} w(y)w(y')k(y,y') - 2\sum_{x\in D}\sum_{y\in E} w(x)w(y)k(x,y)$$

computable

Choice of functions in PWGK

$$\begin{array}{ccc} \mathcal{D} & \longrightarrow & \mathcal{H}_k \\ \Downarrow & & \Downarrow \\ D & \longmapsto & E_k(\mu_D^w) = \sum_{x \in D} w(x) k(\cdot, x) \end{array}$$

To obtain a RKHS representation, we have used a weight function w and a kernel k. In this talk, we set the following functions:

$$k_G(x, y) = e^{-\frac{\|x-y\|^2}{2\sigma^2}}$$

$$w_{\mathrm{arc}}(x) = \arctan(C\mathrm{pers}(x)^p) \ (C, p > 0)$$

$$\mathrm{pers}(x) = d - b \ (x = (b, d) \in \mathbb{R}^2_{ul})$$

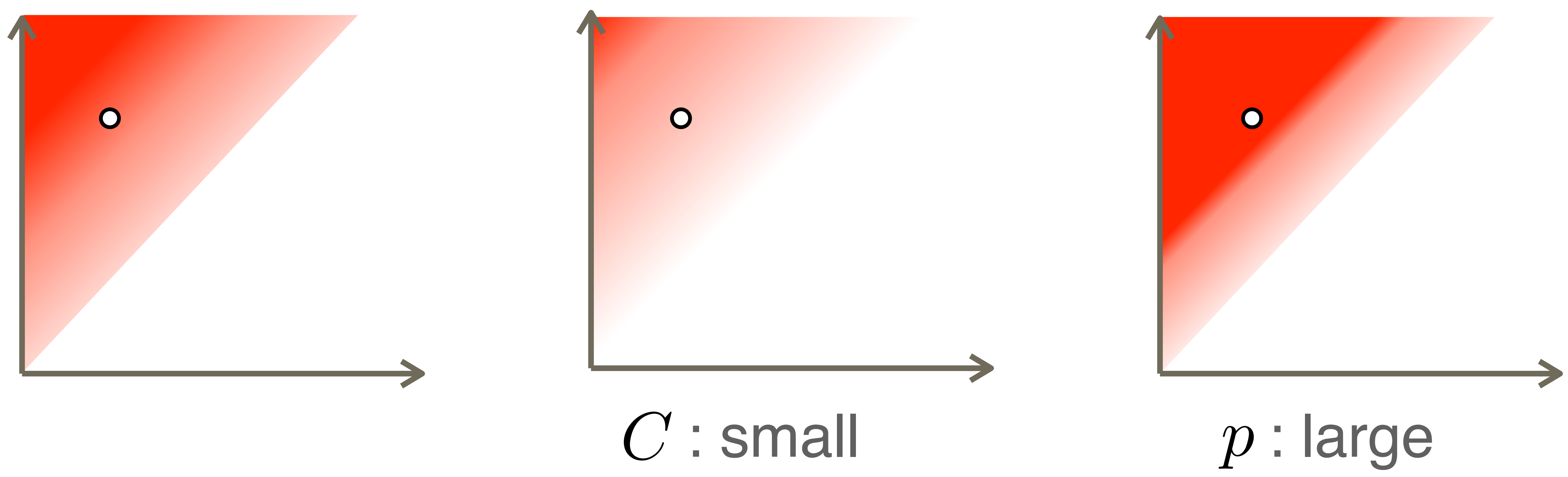
The reason of w_{arc} is for stability result.

Weight function

Parameters appearing $w_{\mathrm{arc}}(x) = \arctan(C \mathrm{pers}(x)^p)$ control

C : where is a noisy region,

p : how sharp is the noisy decision boundary.



Strong (light) red mean that the value of weight function is high (low).

Stability theorem

Main theorem [K, Fukumizu, Hiraoka, 2016]

For a compact subset $M \subset \mathbb{R}^d$ and two finite point sets X, Y in M, if $p > d+1$, then

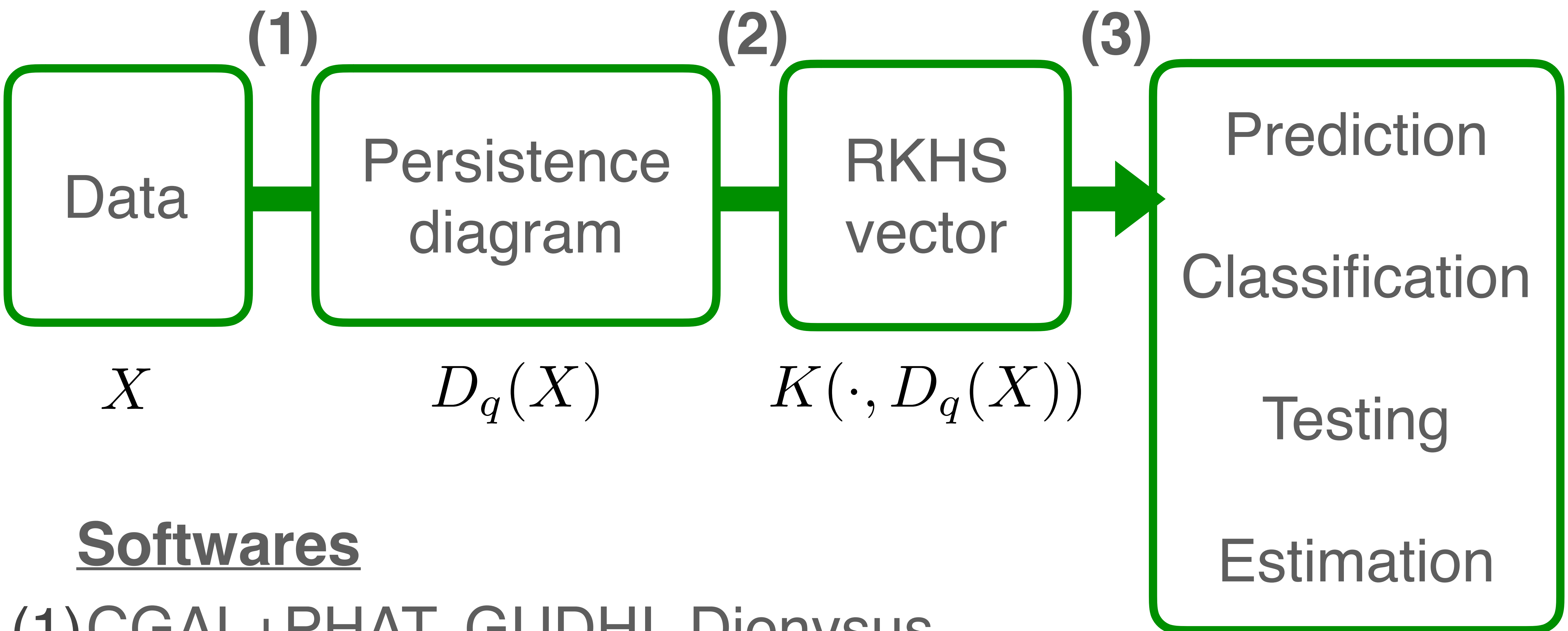
$$\left\| E_{k_G}(\mu^{w_{\mathrm{arc}}}_{D_q(X)}) - E_{k_G}(\mu^{w_{\mathrm{arc}}}_{D_q(Y)}) \right\|_{\mathcal{H}_{k_G}} \leq L(M,d;C,p,\sigma) d_B(D_q(X), D_q(Y)) \; ,$$

where

$$L(M,d;C,p,\sigma) = \left\{ \frac{\sqrt{2}}{\sigma} \frac{p}{p-d} C_M \mathrm{diam}(M)^{p-d} + \frac{4p(p-1)}{p-1-d} C_M \mathrm{diam}(M)^{p-1-d} \right\} C \; .$$

- Kernel embedding $D \mapsto \sum_{x \in D} w(x) k(\cdot, x)$ is **injective** and **continuous** (k_G is a C_0-universal kernel)

Statistical Topological Data Analysis



Softwares

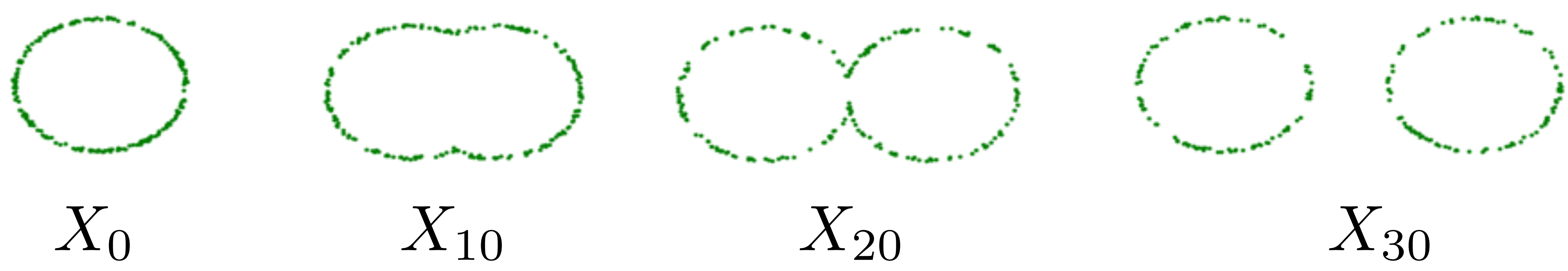
(1) CGAL+PHAT, GUDHI, Dionysus, R-TDA, Ripser, **HomCloud**(Hiraoka lab), …

(2) Kernel on persistence diagrams (This work)

(3) libsvm, e-1071, scikit-learn, …

Section 4
Demonstrations

Synthesized two circles data



$$d = 0.05k \ (k = 0, \cdots, 40)$$

$$\begin{cases} x_1(i) &= \cos(t_1^i) - d \\ y_1(i) &= \sin(t_1^i) \end{cases} \qquad t_1^i \sim \begin{cases} [\arccos(d), 2\pi - \arccos(d)] \ (d < 1) \\ [0, 2\pi] \ (d > 1) \end{cases}$$

$$\begin{cases} x_2(i) &= \cos(t_2^i) + d \\ y_2(i) &= \sin(t_2^i) \end{cases} \qquad t_2^i \sim \begin{cases} [-\pi + \arccos(d), \pi - \arccos(d)] \ (d < 1) \\ [-\pi, \pi] \ (d > 1) \end{cases}$$

$$X_k := \{(x_1(i), y_1(i))\}_{i=1,\cdots,100} \cup \{(x_2(i), y_2(i))\}_{i=1,\cdots,100}$$

Goal : Detect the change point in this system

Procedures

1. **Prepare data (two circles data)**

$$X_1, \cdots, X_n$$

2. **Compute persistence diagrams**

$$D(X_1), \cdots, D(X_n)$$

3. **Compute the Gram matrix**

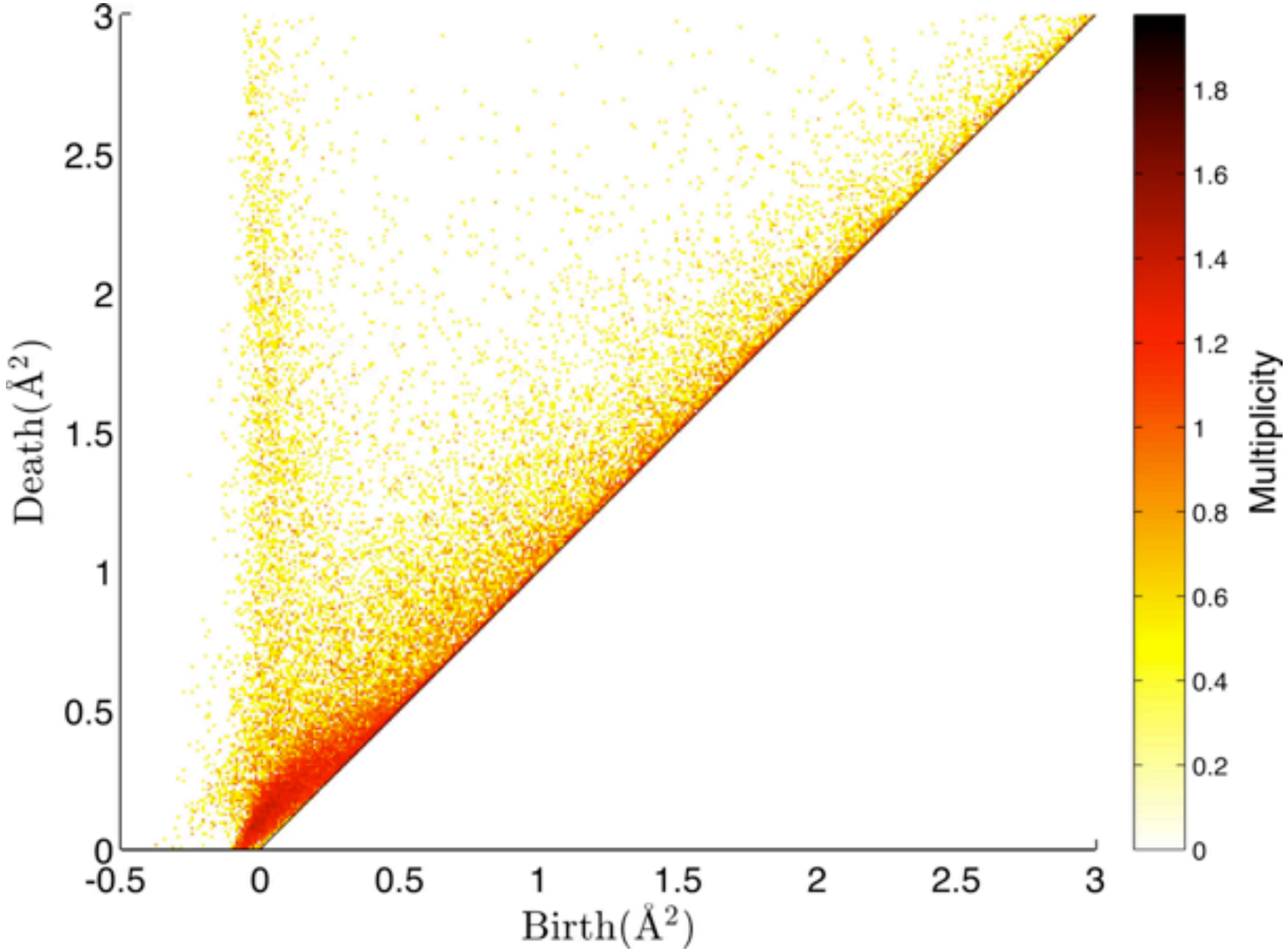
$$K_G(D(X_i), D(X_j)) = \exp\left(-\frac{1}{2\tau^2}\left\|E_k(\mu^w_{D(X_i)}) - E_k(\mu^w_{D(X_j)})\right\|^2_{\mathcal{H}_k}\right)$$

4. **Apply statistical methods**
   kernel change point analysis
   kernel principal component analysis (kPCA)

Section 5
Applications

Application for glass transition problem

Data are atomic configurations of silica obtained from several temperatures (from liquid to glass).



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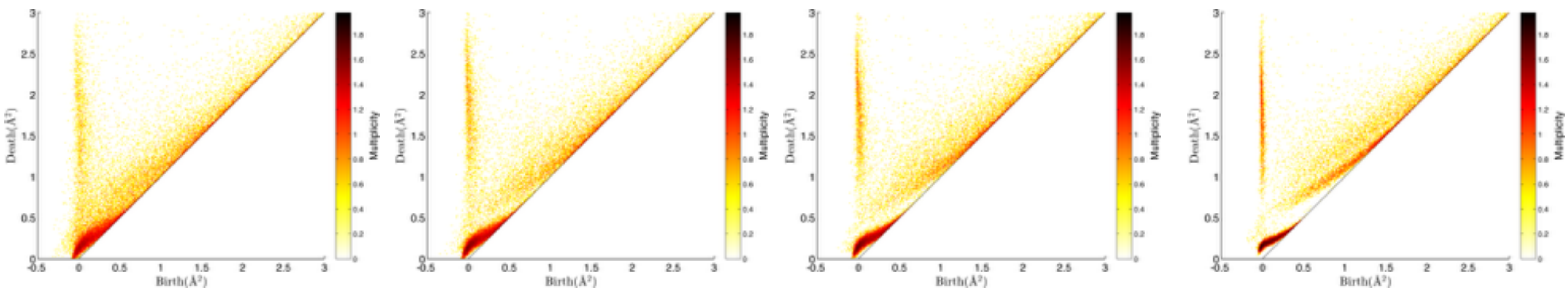
Data are atomic configurations of silica obtained from several temperatures.

$D_1 \quad \cdots \quad D_\ell \qquad D_{\ell+1} \quad \cdots \quad D_{80}$



Liquid ⟷ Glass

Where (which index ℓ) is a transition point?

What we have to do is just to compute the Gram matrix of persistence diagrams $(K(D_i, D_j))_{i,j=1,\ldots,n}$ (Kernel method).

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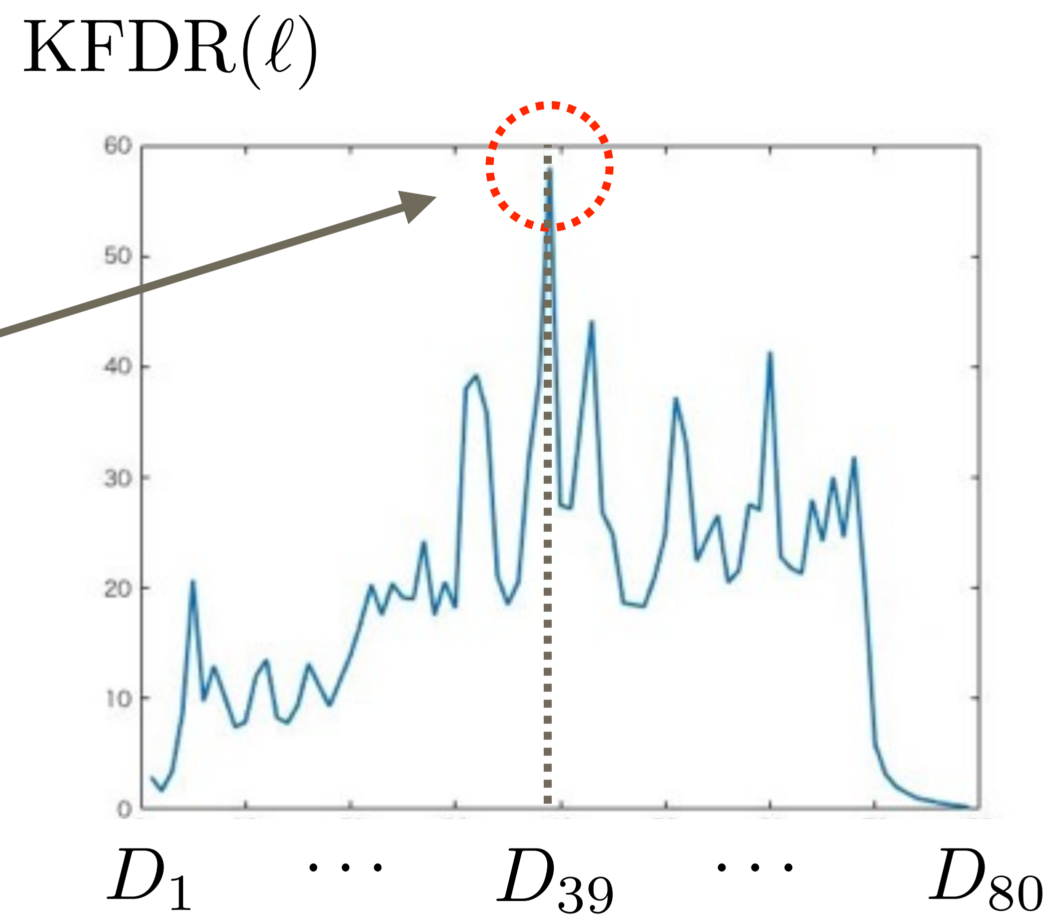

The change point is estimated from the peak of the KFDR graph.

This KFDR result tells us that $D_{39} \simeq 3100\mathrm{K}$ is an estimated change point and it is in the liquid-glass transition interval $[2000\mathrm{K}, 3500\mathrm{K}]$ which is determined by physics.

Remark: Our method uses only topological structure of silica.

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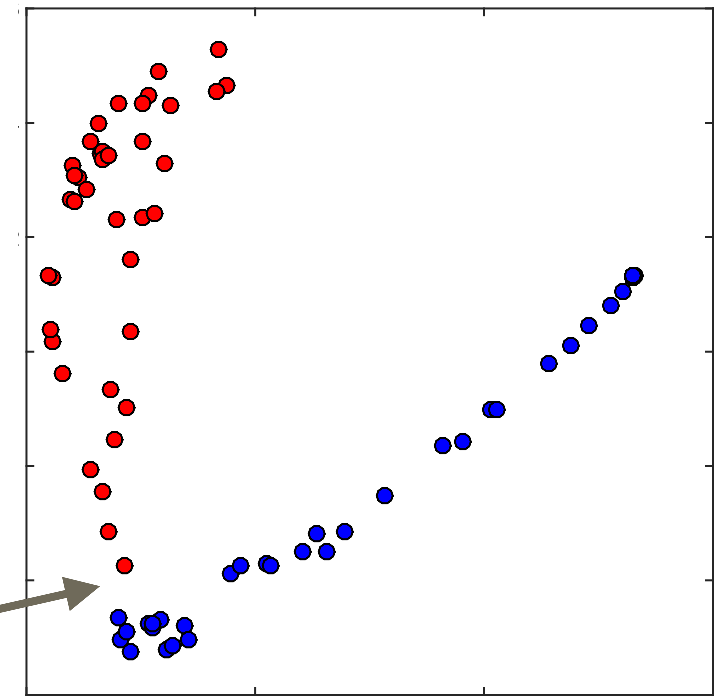
3100K



Contribution rate : 81.9%

The 2-dimensional kernel principal component analysis (PCA) plot of persistence diagrams and colors are assigned before and after $3100\mathrm{K}$.

Conclusion

Our contribution : Kernel based statistical framework on persistence diagram

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Reference

G. Kusano, Kenji Fukumizu, and Yasuaki Hiraoka. Persistence weighted Gaussian kernel for topological data analysis, ICML, pp. 2004–2013, 2016.

Thank you for your attention