Geiranger, Norway - June 5, 2018
Abel Symposium

The density of expected persistence diagrams and its kernel based estimation

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(Joint work with Vincent Divol)

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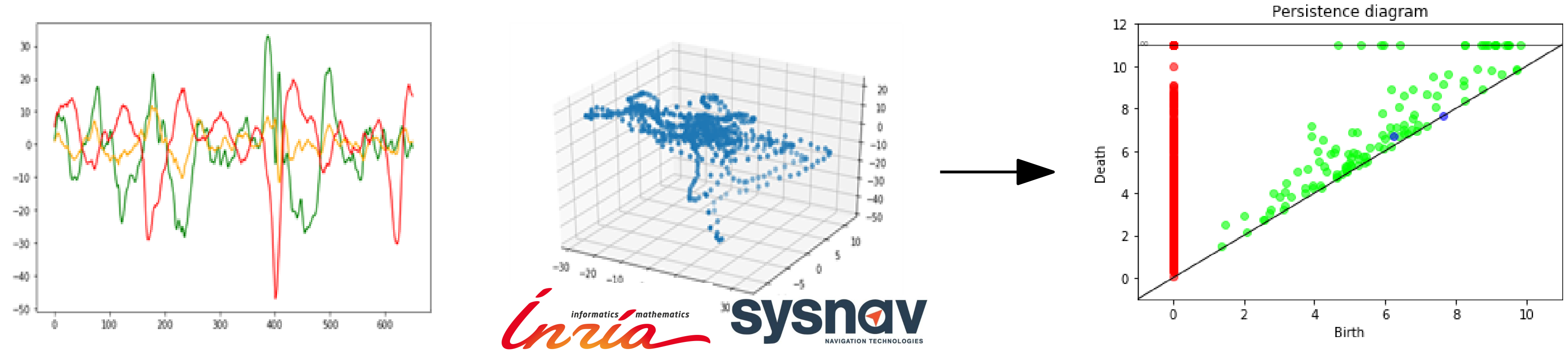
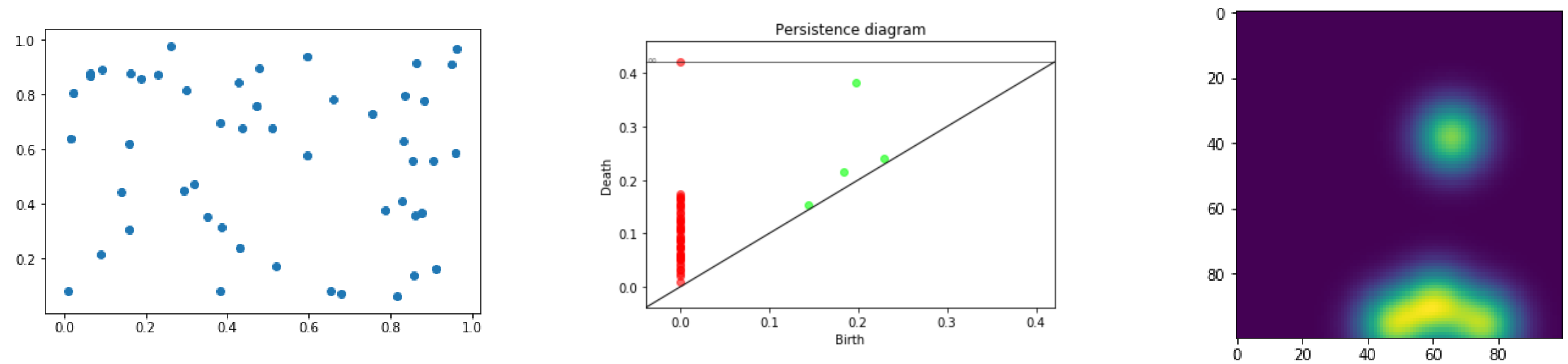
Introduction and motivation





[Persist. surf., Adams et al, 2017]

In many TDA applications :

- persistence diagrams come as distributions (e.g., one diagram per observation).
- persistence information is used through "persistence representations" (vectors, curves, images,...).

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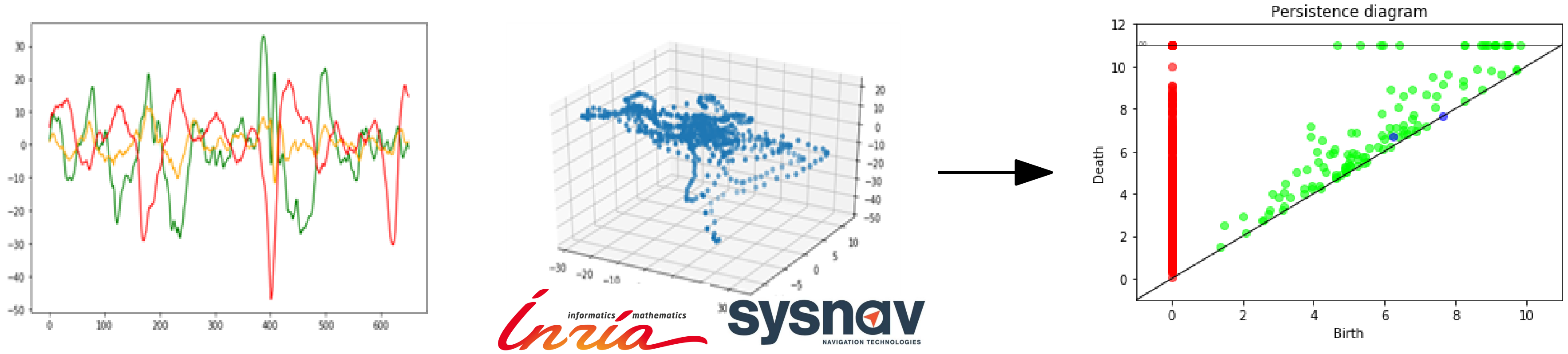

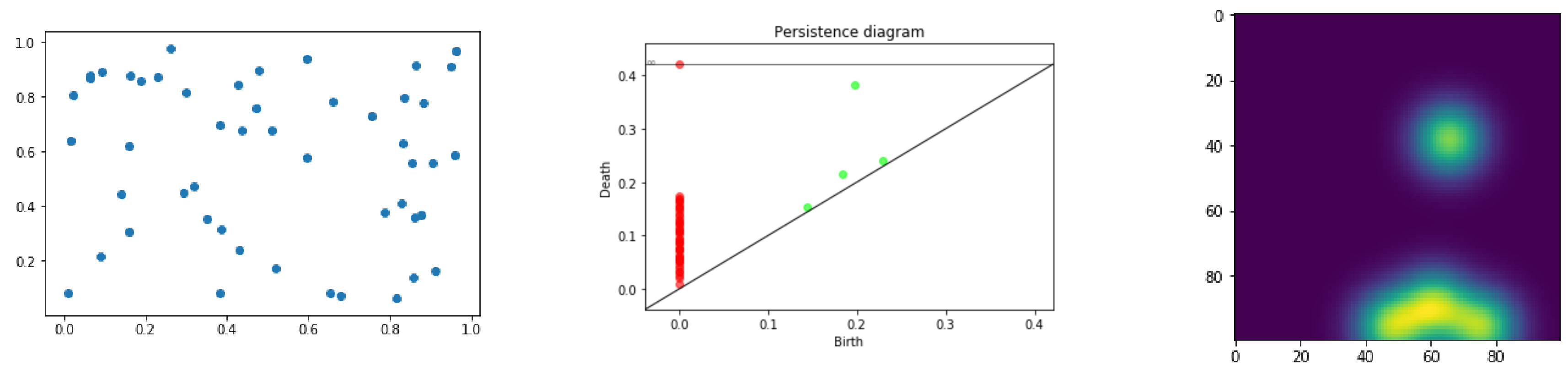

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In many TDA applications :

- persistence diagrams come as distributions (e.g., one diagram per observation).
- persistence information is used through "persistence representations" (vectors, curves, images,...).

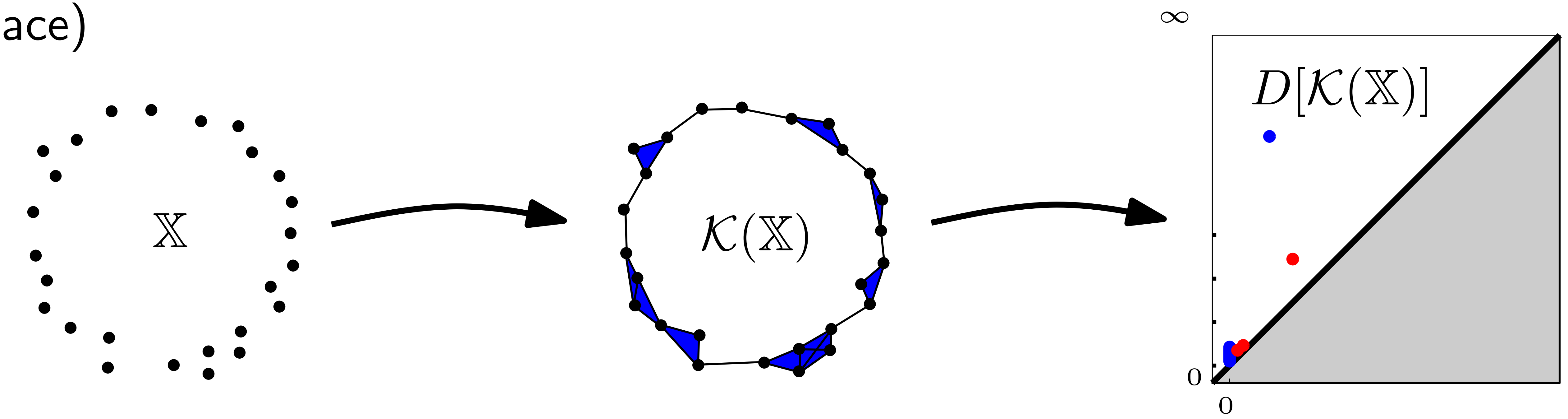
Goal : Understand the statistical behavior of these distributions and representations.

Statistical setting

$\mathbb{X}$ is a random point coud (in some metric space)

$\mathcal{K}$ is a deterministic filtration (e.g. Rips)

$D[\mathcal{K}(\mathbb{X})]$ becomes random



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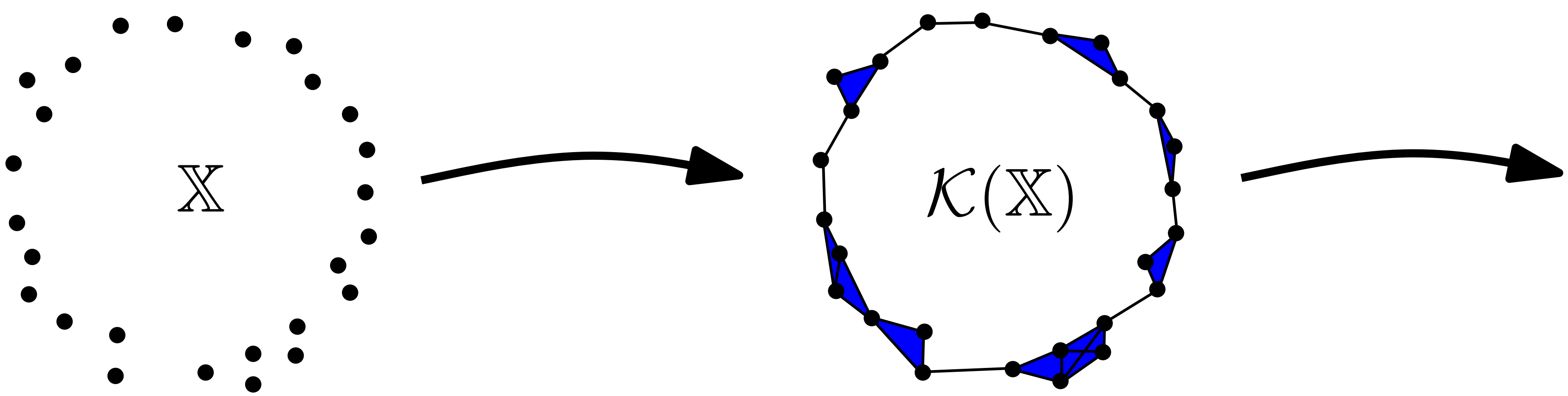

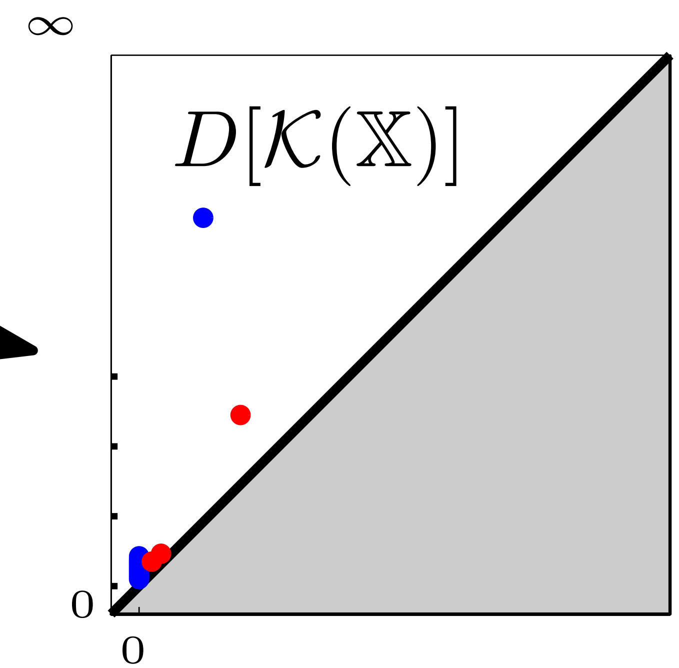

What can be said about the distribution of diagrams $D[\mathcal{K}(\mathbb{X})]$?

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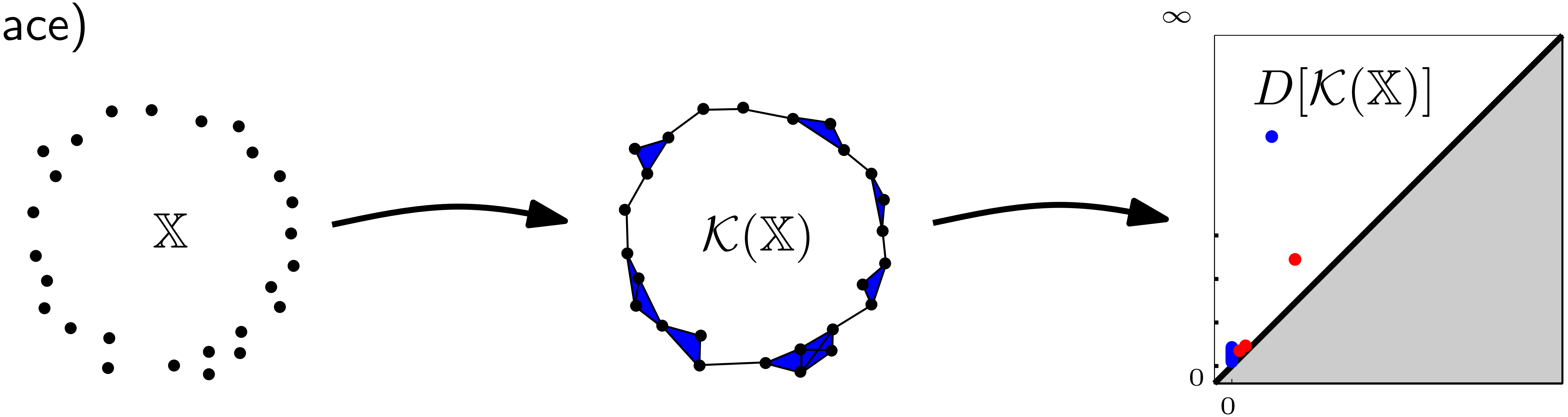
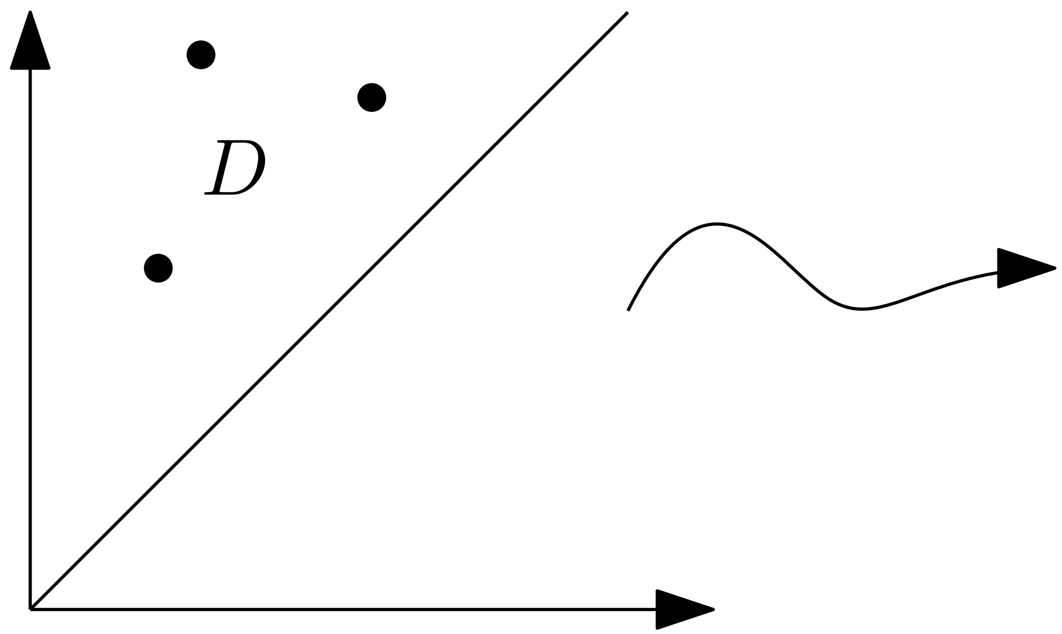


What can be said about the distribution of diagrams $D[\mathcal{K}(\mathbb{X})]$?

Understand the structure of $E[D[\mathcal{K}(\mathbb{X})]]$ in the non asymptotic setting ($|\mathbb{X}| = n$ is fixed, or bounded)

What does this mean ?

Persistence diagrams as discrete measures



$$D := \sum_{\mathbf{r} \in D} \delta_{\mathbf{r}}$$

Motivations :

- The space of measures is much nicer that the space of P. D. !
- In the "standard" algebraic persistence theory, persistence diagrams naturally appear as discrete measures in the plane (over rectangles).
  [Chazal, de Silva, Glisse, Oudot 16]
- Many persistence representations can be expressed as

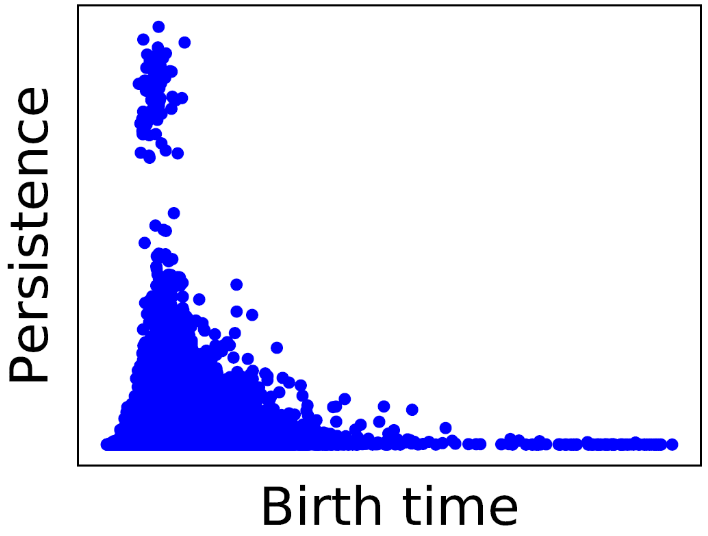
$$D(\phi) = \sum_{\mathbf{r} \in D} \phi(\mathbf{r}) = \int \phi(\mathbf{r}) dD(\mathbf{r})$$

for well-chosen functions ϕ.

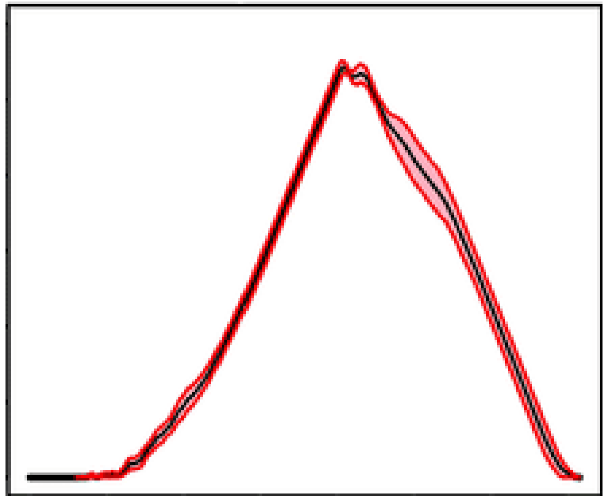
Representation of Persistence diagrams

A representation is called linear if there exists $\phi : \mathbb{R}^2_> \to \mathcal{H}$ such that

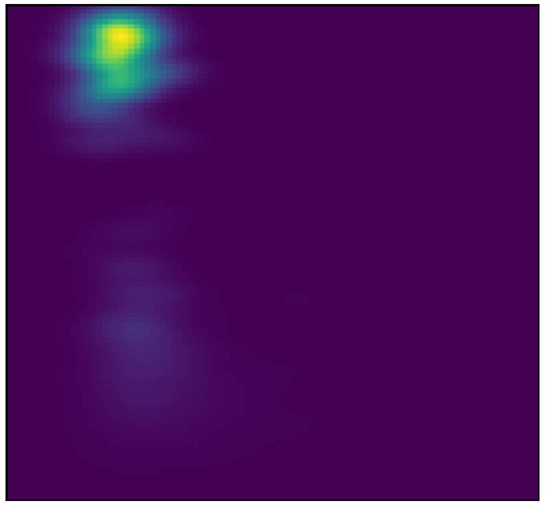
$$\Phi(D) = \sum_{\mathbf{r} \in D} \phi(r) := D(\phi) = \int \phi(\mathbf{r})\, dD(\mathbf{r})$$



Distrib. of life span, total persistence,...



Persistent silhouette
[Chazal & al, 2013]



Persistent surface
[Adams & al, 2016]

Representation of Persistence diagrams

— D is a random persistence diagram (coming from some phenomenon).
— $E[D]$ is a deterministic measure on $\mathbb{R}^2_>$ defined by

$$\forall A \subset \mathbb{R}^2_>,\ E[D](A) = E[D(A)].$$

— $D_1, \ldots, D_N$ i.i.d.

$$\begin{aligned} \overline{\Phi} &= \frac{\Phi(D_1) + \cdots + \Phi(D_N)}{N} \\ &= \overline{\mu}(\phi) \\ &\approx E[D](\phi) \\ E[D](\phi) &= \int_{\mathbb{R}^2_>} \phi(\mathbf{r}) p(\mathbf{r}) d\,\mathbf{r} \quad ? \end{aligned}$$

Does $E[D]$ has a density w.r.t. Lebesgue measure in $\mathbb{R}^2$?
Estimation of p ?

Persistent homology of filtered simplicial complexes

Let $\mathbb{S} = (\mathbb{S}_a \mid a \in \mathbf{R})$ be a finite filtered simplicial complex with N simplicices and let $\mathbb{S}_{a_1} \subset \mathbb{S}_{a_2} \subset \cdots \subset \mathbb{S}_{a_N}$ be the discrete filtration induced by the entering times of the simplices : $\mathbb{S}_{a_i} \setminus \mathbb{S}_{a_{i-1}} = \sigma_{a_i}$.

Persistence algorithm :

1. Process the simplices according to their order of entrance in the filtration.
2. Pairs simplices $(\sigma_{a_j}, \sigma_{a_i})$.
3. Create points (a_j, a_i) in the persistence diagram.

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Important to remember : the persistence pairs are determined by the order on the simplices ; the corresponding points in the diagrams are determined by the filtering values.

Filtrations revisited

Let $n > 0$ be an integer,
$\mathcal{F}_n$: the collection of non-empty subsets of $\{1, \ldots, n\}$,
M : a real analytic compact d-dim. connected manifold (poss. with boundary).

Filtering function :

$$\varphi = (\varphi[J])_{J \in \mathcal{F}_n} : M^n \to \mathbb{R}^{|\mathcal{F}_n|}$$

satisfiying the following conditions :

(K2) *Invariance by permutation :* For $J \in \mathcal{F}_n$ and for $(x_1, \ldots, x_n) \in M^n$, if τ is a permutation of the entries having support included in J, then $\varphi[J](x_{\tau(1)}, \ldots, x_{\tau(n)}) = \varphi[J](x_1, \ldots, x_n)$.

(K3) *Monotony :* For $J \subset J' \in \mathcal{F}_n$, $\varphi[J] \leq \varphi[J']$.

Given $x = (x_1, \cdots, x_n)$, $\varphi(x)$ induces an order on the faces of the simplex with n vertices that is a filtration $\mathcal{K}(x)$:

$$\forall J \in \mathcal{F}_n,\ J \in \mathcal{K}(x, r) \Longleftrightarrow \varphi[J](x) \leq r.$$

Filtrations revisited

Not : for $x = (x_1, \ldots, x_n) \in M^n$ and for J a simplex, $x(J) := (x_j)_{j \in J}$

(K1) *Absence of interaction :* For $J \in \mathcal{F}_n$, $\varphi[J](x)$ only depends on $x(J)$.

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(K5) *Smoothness :* The function φ is subanalytic and the gradient of each of its entries (which is defined a.s.e.) is non vanishing a.s.e..

The example of the Vietoris-Rips filtration

$$\varphi[J](x) = \max_{i,j \in J} d(x_i, x_j)$$

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The density of expected persistence diagrams

Theorem : Fix $n \geq 1$. Assume that :

- M is a real analytic compact d-dimensional connected submanifold possibly with boundary,
- $\mathbb{X}$ is a random variable on M^n having a density with respect to the Haussdorf measure $\mathcal{H}_{dn}$,
- $\mathcal{K}$ satisfies the assumptions (K1)-(K5).

Then, for $s \geq 0$, $E[D_s[\mathcal{K}(\mathbb{X})]]$ has a density with respect to the Lebesgue measure on the half plane $\mathbb{R}^2_> = \{(b, d) \in \mathbb{R}^2 : b \leq d\}$.

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Then, for $s \geq 1$, $E[D_s[\mathcal{K}(\mathbb{X})]]$ has a density with respect to the Lebesgue measure on $\mathbb{R}^2_>$. Moreover, $E[D_0[\mathcal{K}(\mathbb{X})]]$ has a density with respect to the Lebesgue measure on the vertical line $\{0\} \times [0, \infty)$.

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Technical assumption (related to finiteness properties of subanalytic sets) that can be discarded in most cases.

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Theorem [smoothness] : Under the assumption of previous theorem, if moreover $\mathbb{X} \in M^n$ has a density of class C^k with respect to $\mathcal{H}_{nd}$. Then, for $s \geq 0$, the density of $E[D_s[\mathcal{K}(\mathbb{X})]]$ is of class C^k.

Sketch of proof

1. There exists a partition of the complement of a (subanalytic) set of measure 0 in M^n by open sets $V_1, \cdots, V_R$ such that :

- the order of the simplices of $\mathcal{K}(x)$ is constant on each V_r,
- for any $r = 1, \cdots, R$, and any $x \in V_r$,

$$D_s[\mathcal{K}(x)] = \sum_{i=1}^{N_r} \delta_{\mathbf{r}_i}$$

  with $\mathbf{r}_i = (\varphi[J_{i_1}](x), \varphi[J_{i_2}](x))$ where N_r, J_{i_1}, J_{i_2} only depends on V_r.
- J_{i_1}, J_{i_2} can be chosen so that the differential of

$$\Phi_{ir} : x \in V_r \to \mathbf{r}_i = (\varphi[J_{i_1}](x), \varphi[J_{i_2}](x))$$

  has maximal rank (2).

Sketch of proof

2. The expected diagram can be written as

$$\begin{aligned} E[D_s[\mathcal{K}(\mathbb{X})]] &= \sum_{r=1}^{R} E\left[\mathbb{1}\{\mathbb{X} \in V_r\} D_s[\mathcal{K}(\mathbb{X})]\right] = \sum_{r=1}^{R} E\left[\mathbb{1}\{\mathbb{X} \in V_r\} \sum_{i=1}^{N_r} \delta_{\mathbf{r}_i}\right] \\ &= \sum_{r=1}^{R} \sum_{i=1}^{N_r} E\left[\mathbb{1}\{\mathbb{X} \in V_r\} \delta_{\mathbf{r}_i}\right] \end{aligned}$$

The Hausdorff measure and the co-area formula

Definition : Let k be a non-negative number. For $A \subset \mathbb{R}^D$, and $\delta > 0$, consider

$$\mathcal{H}_k^\delta(A) := \inf \left\{ \sum_i \text{diam}(U_i)^k, A \subset \bigcup_i U_i \text{ and } \text{diam}(U_i) < \delta \right\}.$$

The *k-dimensional Haussdorf measure* on $\mathbb{R}^D$ of A is defined by $\mathcal{H}_k(A) := \lim_{\delta \to 0} \mathcal{H}_k^\delta(A)$.

Theorem [Co-area formula] : Let M (resp. N) be a smooth Riemannian manifold of dimension m (resp n). Assume that $m \geq n$ and let $\Phi : M \to N$ be a differentiable map. Denote by $D\Phi$ the differential of Φ. The Jacobian of Φ is defined by $J\Phi = \sqrt{\det((D\Phi) \times (D\Phi)^t)}$. For $f : M \to N$ a positive measurable function, the following equality holds :

$$\int_M f(x) J\Phi(x) d\mathcal{H}_m(x) = \int_N \left(\int_{x \in \Phi^{-1}(\{y\})} f(x) d\mathcal{H}_{m-n}(x) \right) d\mathcal{H}_n(y).$$

Sketch of proof

2. The expected diagram can be written as

$$E[D_s[\mathcal{K}(\mathbb{X})]] = \sum_{r=1}^{R} E\left[\mathbb{1}\{\mathbb{X} \in V_r\} D_s[\mathcal{K}(\mathbb{X})]\right] = \sum_{r=1}^{R} E\left[\mathbb{1}\{\mathbb{X} \in V_r\} \sum_{i=1}^{N_r} \delta_{\mathbf{r}_i}\right]$$

$$= \sum_{r=1}^{R} \sum_{i=1}^{N_r} E\left[\mathbb{1}\{\mathbb{X} \in V_r\} \delta_{\mathbf{r}_i}\right]$$

μ_{ir}

3. Use the co-area formula :

$$\mu_{ir}(B) = P(\Phi_{ir}(\mathbb{X}) \in B, \mathbb{X} \in V_r)$$

$$= \int_{V_r} \mathbb{1}\{\Phi_{ir}(x) \in B\} \kappa(x) d\mathcal{H}_{nd}(x)$$

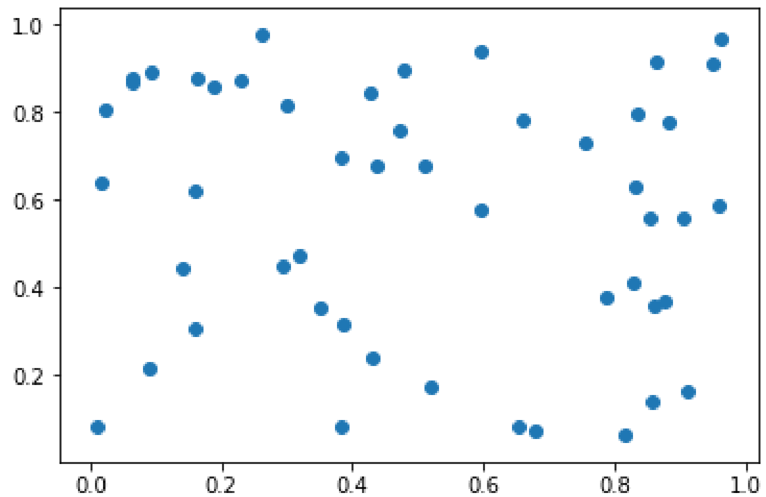
$$= \int_{u \in B} \int_{x \in \Phi_{ir}^{-1}(u)} (J\Phi_{ir}(x))^{-1} \kappa(x) d\mathcal{H}_{nd-2}(x) du.$$

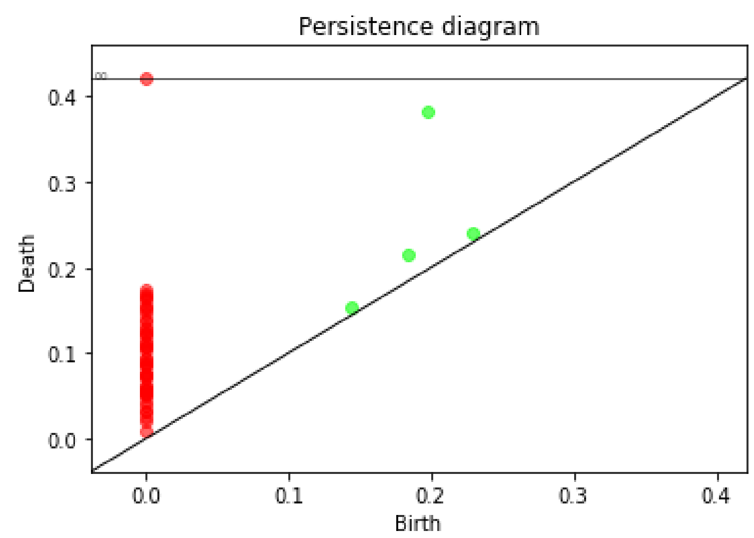
Density of $\mathbb{X}$

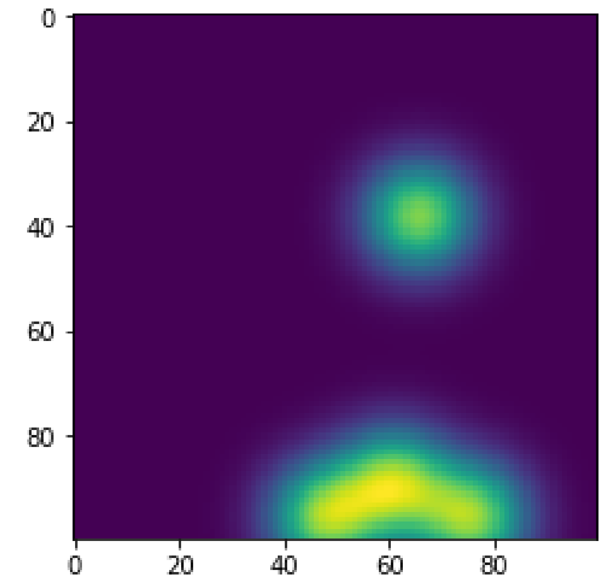
Density of μ_{ir}

Persistence images

[Adams et al, JMLR 2017]







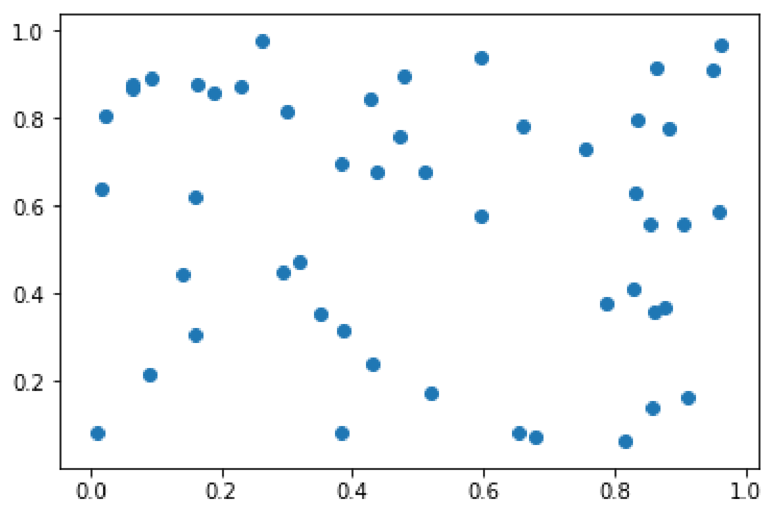
For $K : \mathbb{R}^2 \to \mathbb{R}$ a kernel and H a bandwidth matrix (e.g. a symmetric positive definite matrix), pose for $u \in \mathbb{R}^2$, $K_H(z) = |H|^{-1/2} K(H^{-1/2} \cdot u)$

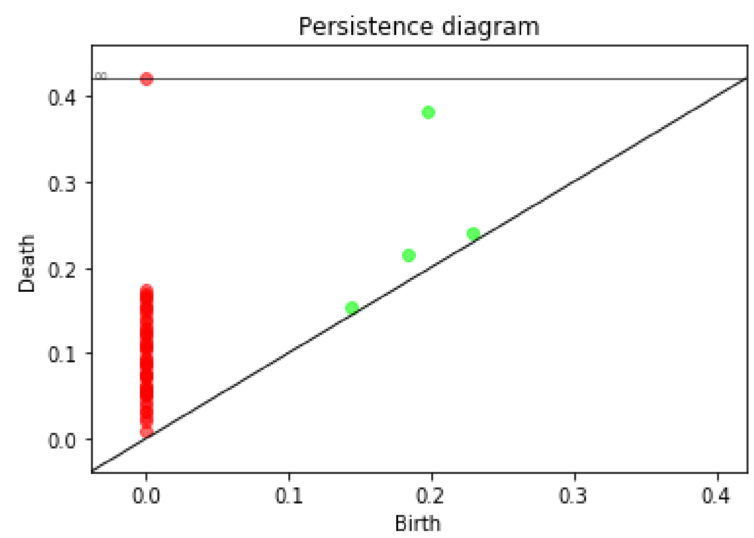
For $D = \sum_i \delta_{\mathbf{r}_i}$ a diagram, $K : \mathbb{R}^2 \to \mathbb{R}$ a kernel, H a bandwidth matrix and $w : \mathbb{R}^2 \to \mathbb{R}_+$ a weight function, one defines the persistence surface of D with kernel K and weight function w by :

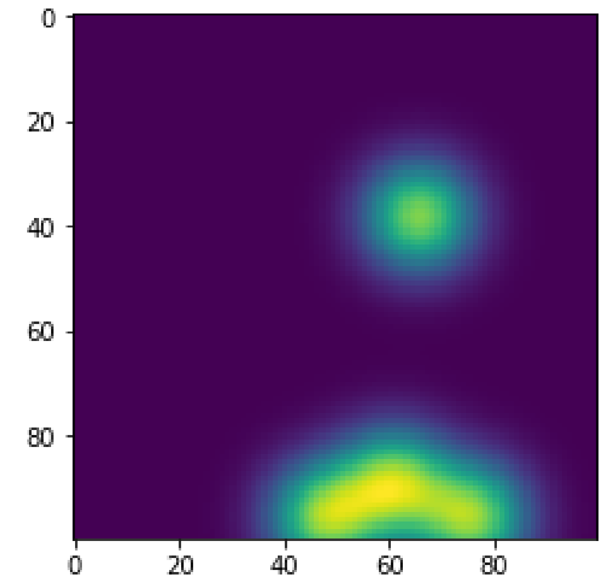
$$\forall z \in \mathbb{R}^2, \ \rho(D)(u) = \sum_i w(\mathbf{r}_i) K_H(u - \mathbf{r}_i) = D(w K_H(u - \cdot))$$

Persistence images

[Adams et al, JMLR 2017]







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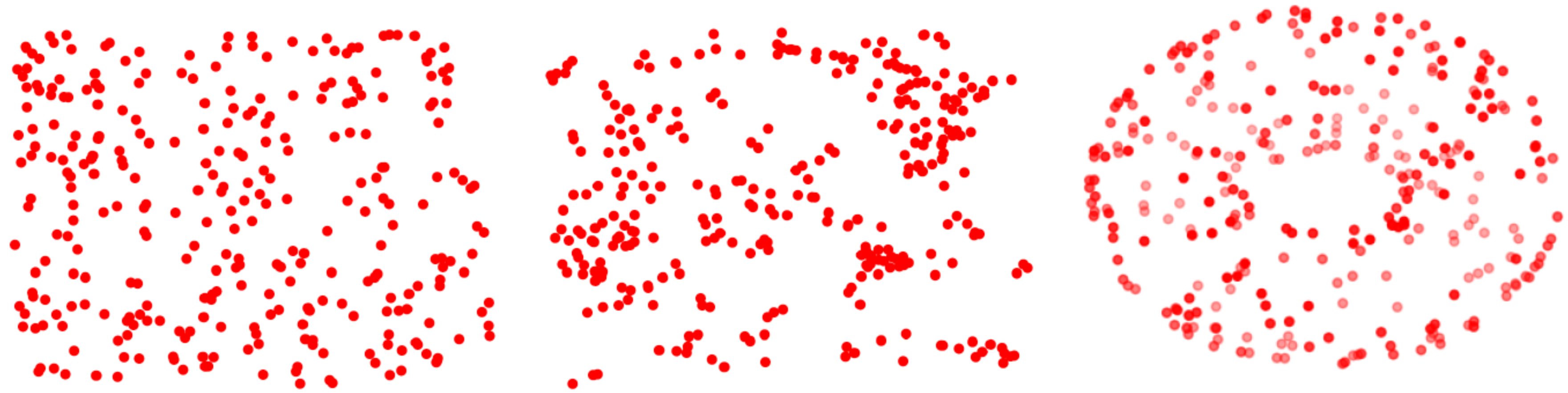
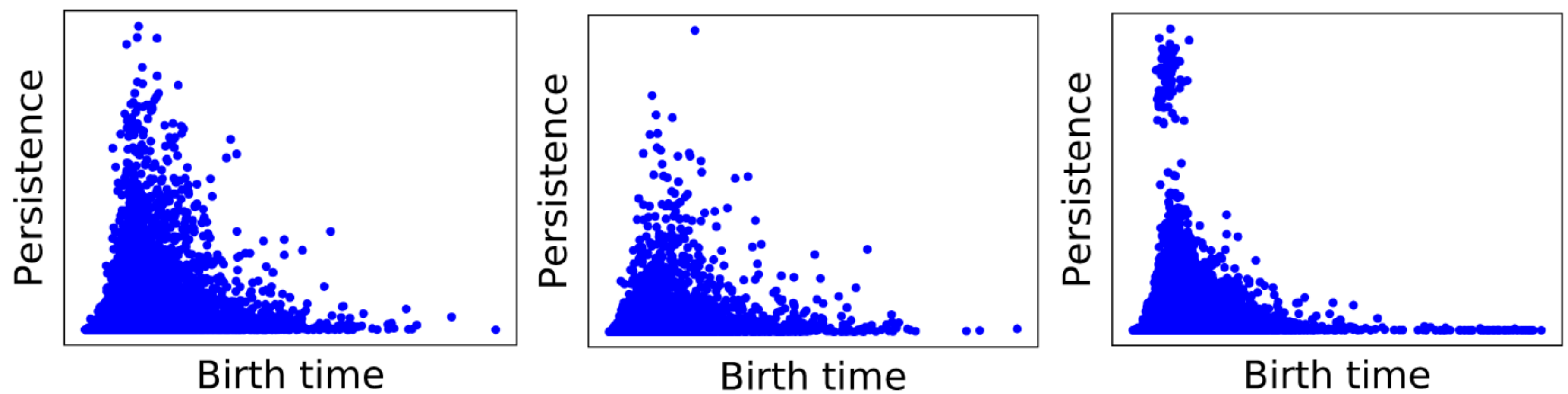
$\Rightarrow$ persistence surfaces can be seen as kernel based estimators of $E[D_s[\mathcal{K}(\mathbb{X})]]$.

Persistence images

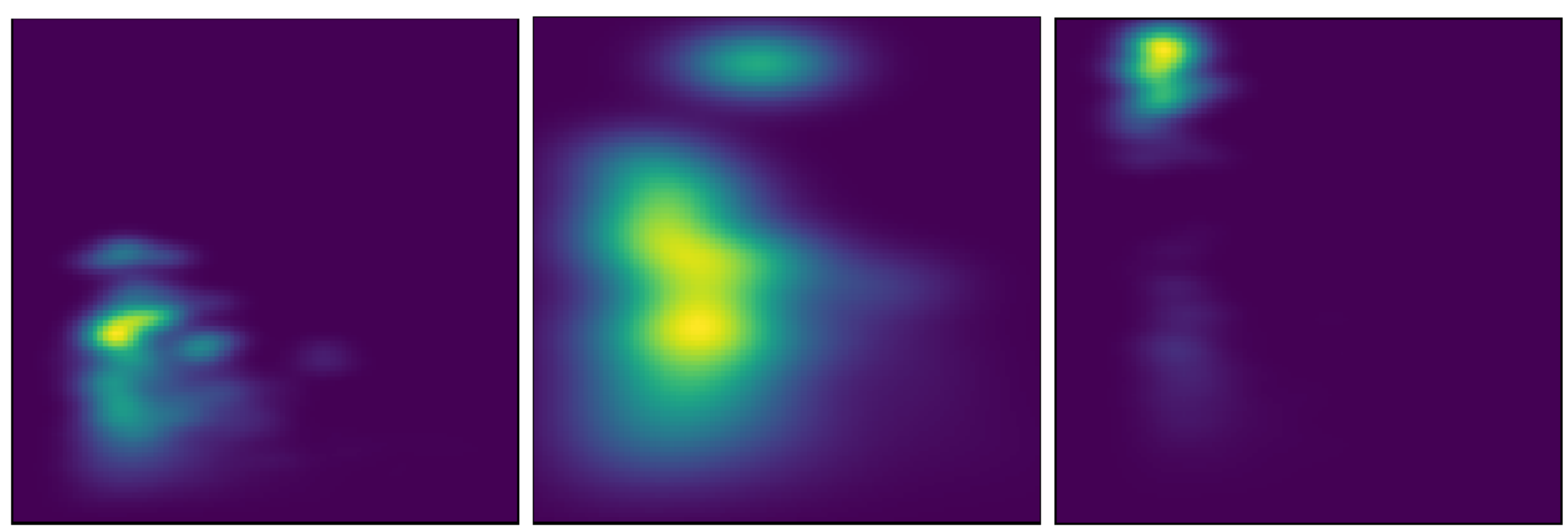
The realization of 3 different processes



The overlay of 40 different persistence diagrams



The persistence images with weight function $w(\mathbf{r}) = (r_2 - r_1)^3$ and bandwith selected using cross-validation.



Thank you for your attention

References :

- F. Chazal, V. Divol, *The density of expected persistence diagrams and its kernel based estimation*, SoCG 2018.

Software :

- GUDHI library C++ / Python : http ://gudhi.gforge.inria.fr/
- R package TDA : Statistical Tools for Topological Data Analysis