On metric and statistical properties of topological descriptors for geometric data

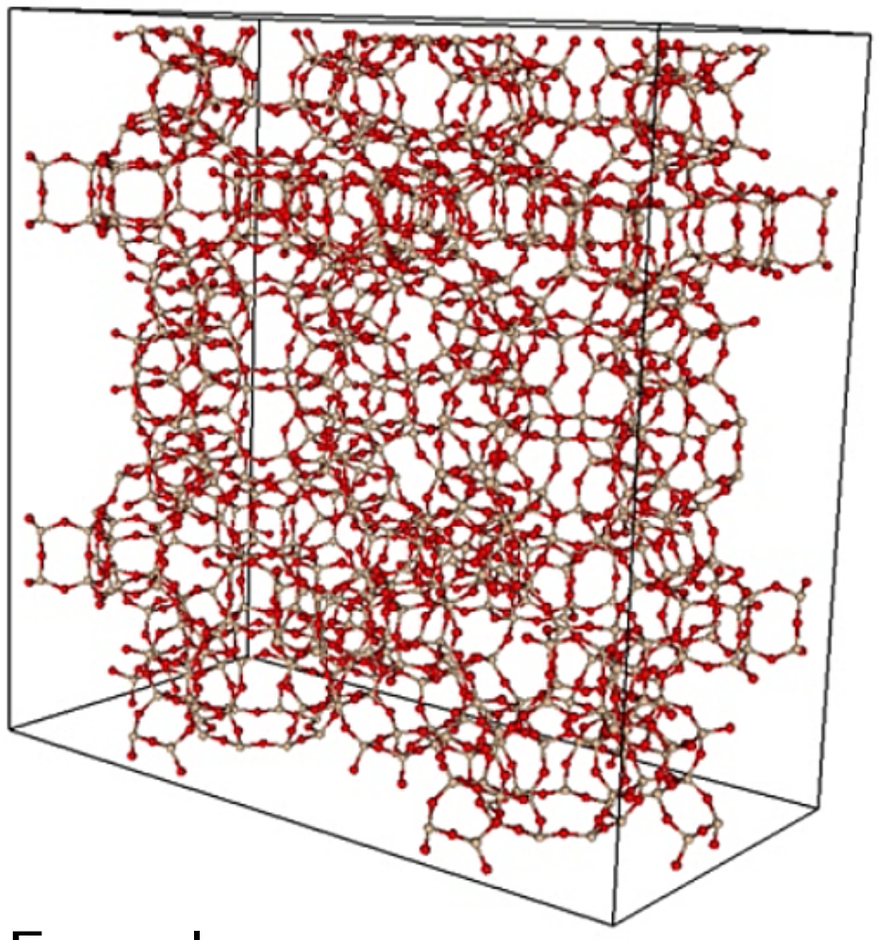
PhD defense of Mathieu Carrière

ÉCOLE DOCTORALE
Sciences et technologies de l'information et de la communication (STIC)

Topological Data Analysis

Modern data sets often have non-trivial underlying structures...

...and these structures (*shapes*) matter



Example:

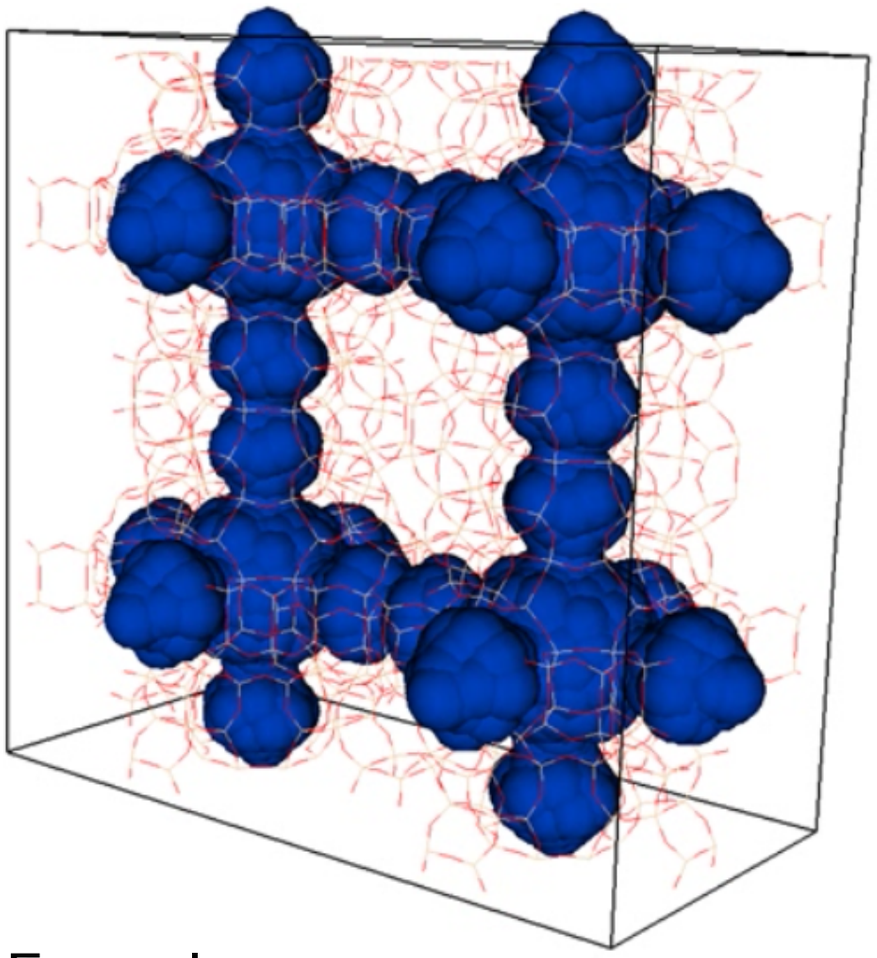
cavities in nanoporous materials
(e.g. zeolites for nanofilters)
determine their physical properties

[Y. Lee et al.: "Quantifying similarity of pore-geometry in nanoporous materials", 2017]

Topological Data Analysis

Modern data sets often have non-trivial underlying structures...

...and these structures (*shapes*) matter



Example:

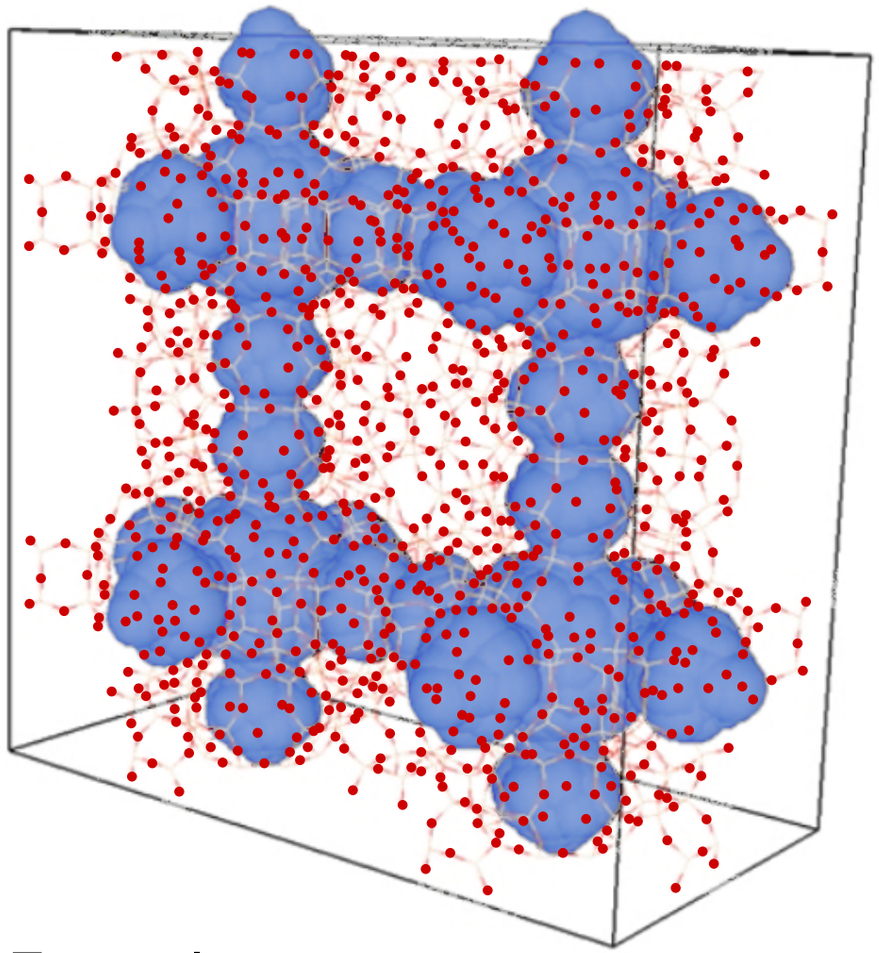
cavities in nanoporous materials
(e.g. zeolites for nanofilters)
determine their physical properties

[Y. Lee et al.: "Quantifying similarity of pore-geometry in nanoporous materials", 2017]

Topological Data Analysis

Modern data sets often have non-trivial underlying structures...

...and these structures (*shapes*) matter



→ need topological descriptors that can:

extract the shapes hidden in data

encode these shapes compactly

Example:

cavities in nanoporous materials
(e.g. zeolites for nanofilters)
determine their physical properties

[Y. Lee et al.: "Quantifying similarity of pore-geometry in nanoporous materials", 2017]

Topological Data Analysis

Why is topology interesting for data analysis?

$\longrightarrow$ multiscale
$\longrightarrow$ compact

Topological Data Analysis

Why is topology interesting for data analysis?

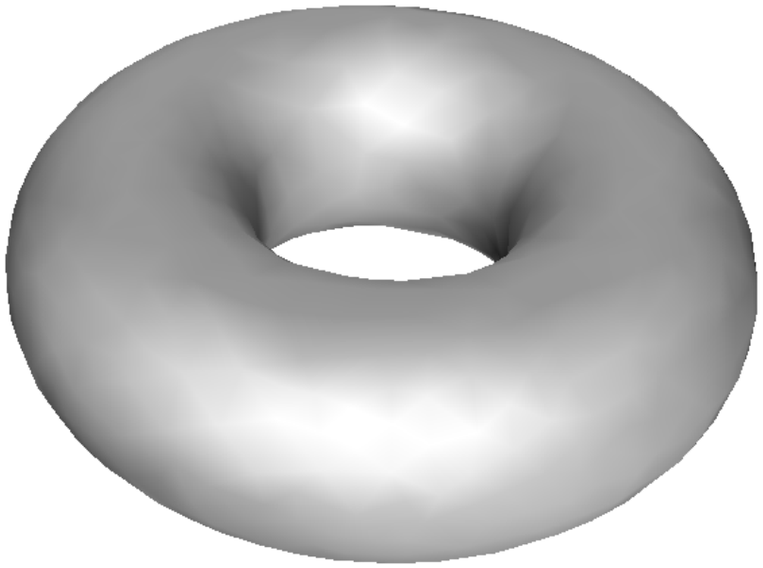
- $\longrightarrow$ multiscale
- $\longrightarrow$ compact
- $\longrightarrow$ complementary to other descriptors
- $\longrightarrow$ stable with respect to (small) perturbations
- $\longrightarrow$ invariant under coordinate changes/rigid transforms

Topological Data Analysis

Why is topology interesting for data analysis?

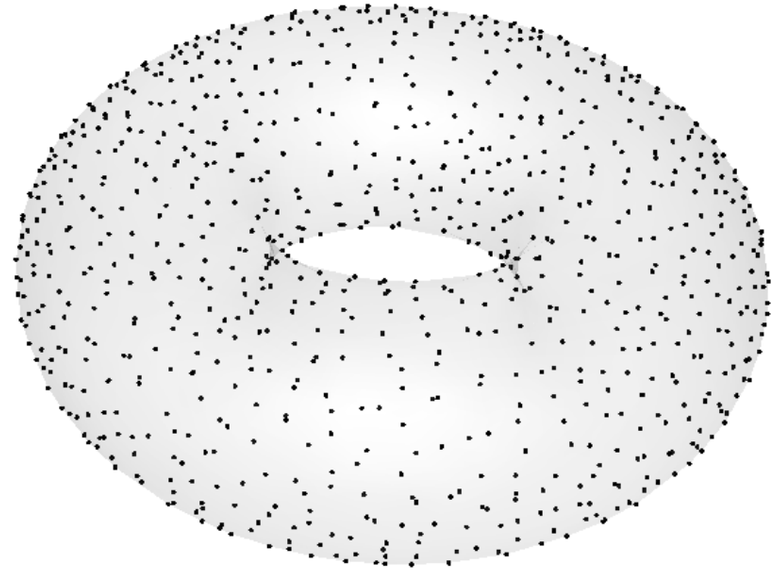
$\longrightarrow$ multiscale
$\longrightarrow$ compact

$\longrightarrow$ complementary to other descriptors
$\longrightarrow$ stable with respect to (small) perturbations
$\longrightarrow$ invariant under coordinate changes/rigid transforms



topological space

topological descriptors



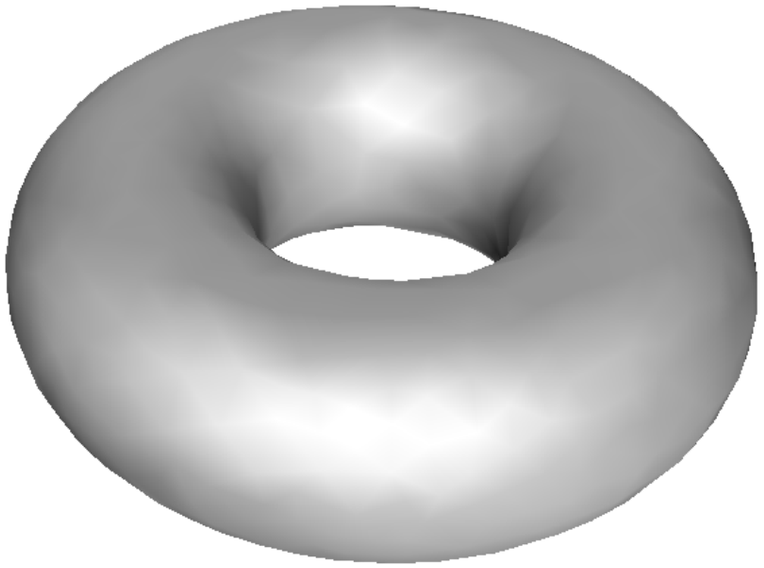
point cloud

Topological Data Analysis

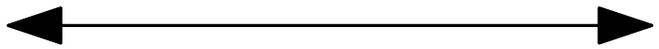
Why is topology interesting for data analysis?

$\longrightarrow$ multiscale
$\longrightarrow$ compact

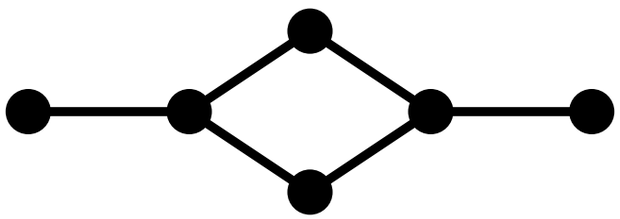
$\longrightarrow$ complementary to other descriptors
$\longrightarrow$ stable with respect to (small) perturbations
$\longrightarrow$ invariant under coordinate changes/rigid transforms

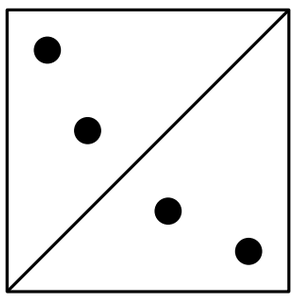


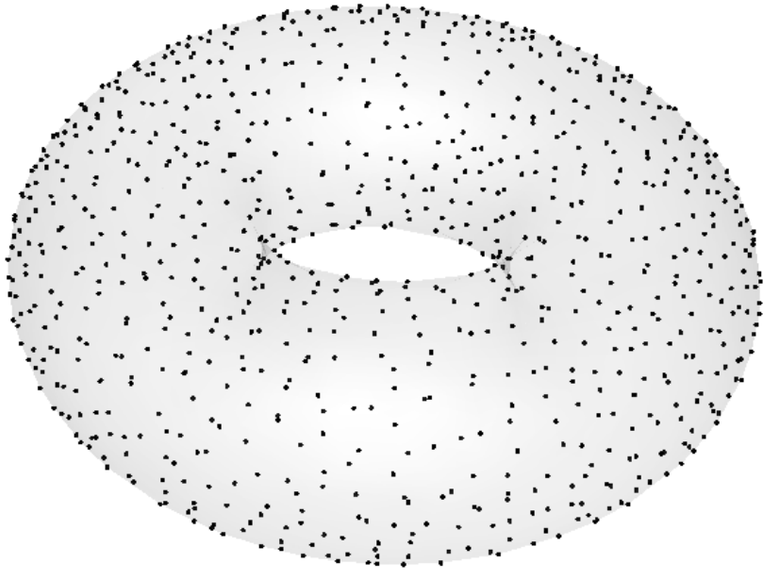
topological space



topological descriptors







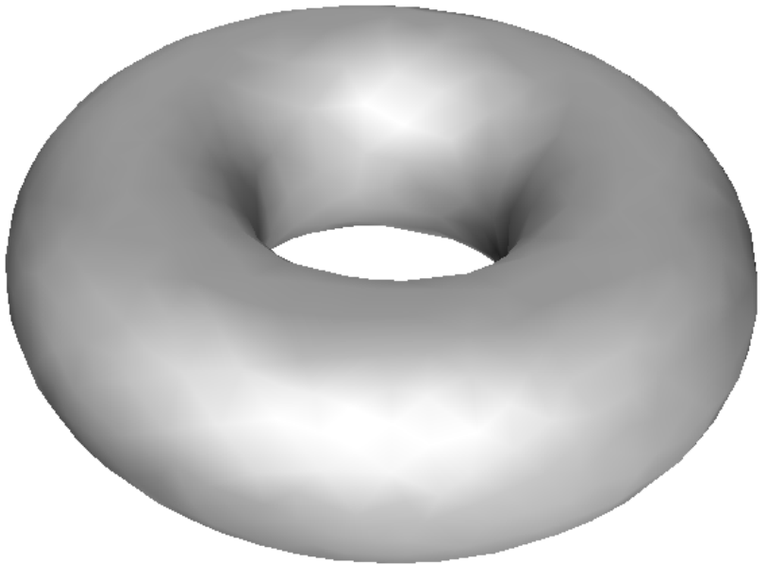
point cloud

Topological Data Analysis

Why is topology interesting for data analysis?

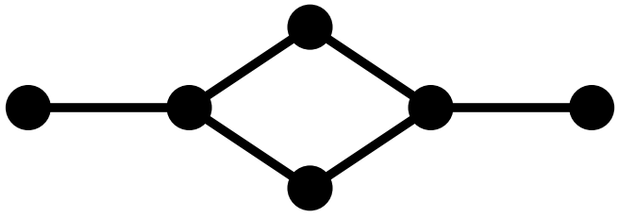
$\longrightarrow$ multiscale
$\longrightarrow$ compact

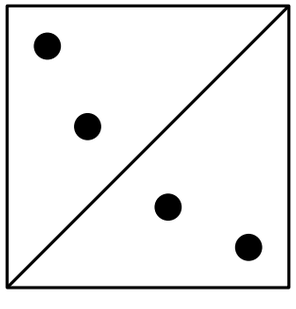
$\longrightarrow$ complementary to other descriptors
$\longrightarrow$ stable with respect to (small) perturbations
$\longrightarrow$ invariant under coordinate changes/rigid transforms

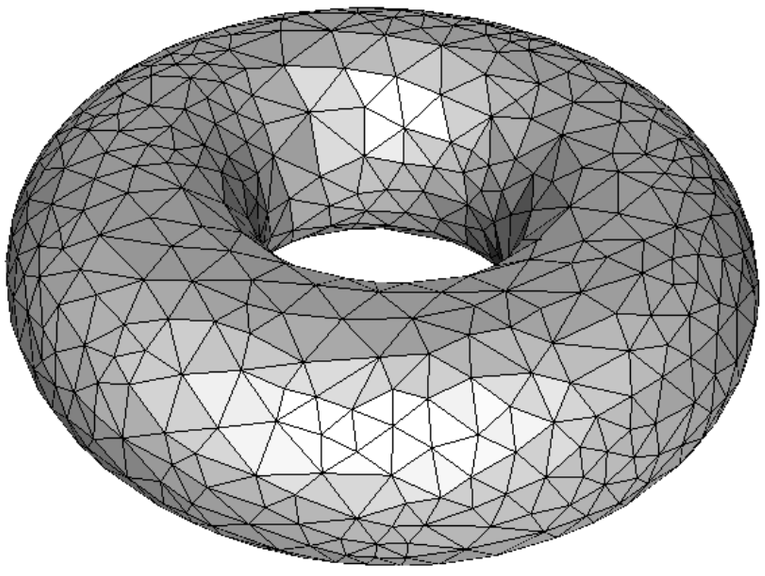


topological space

topological descriptors







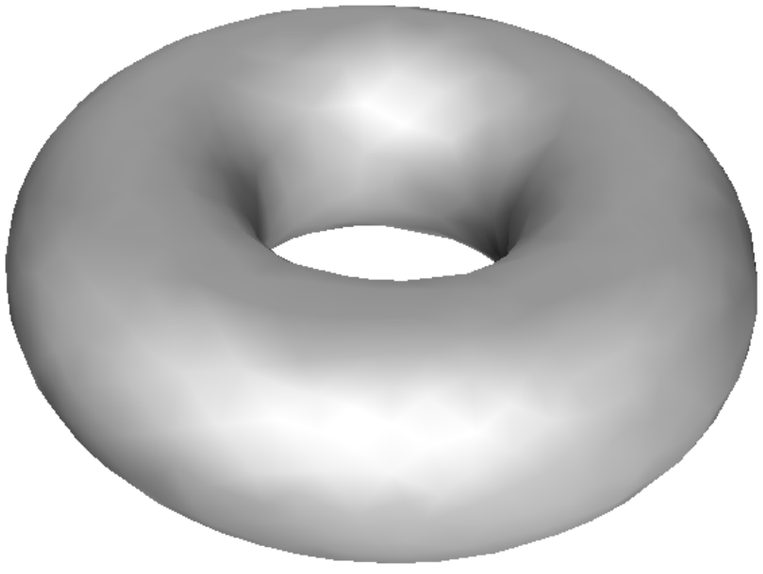
point cloud
triangulation

Topological Data Analysis

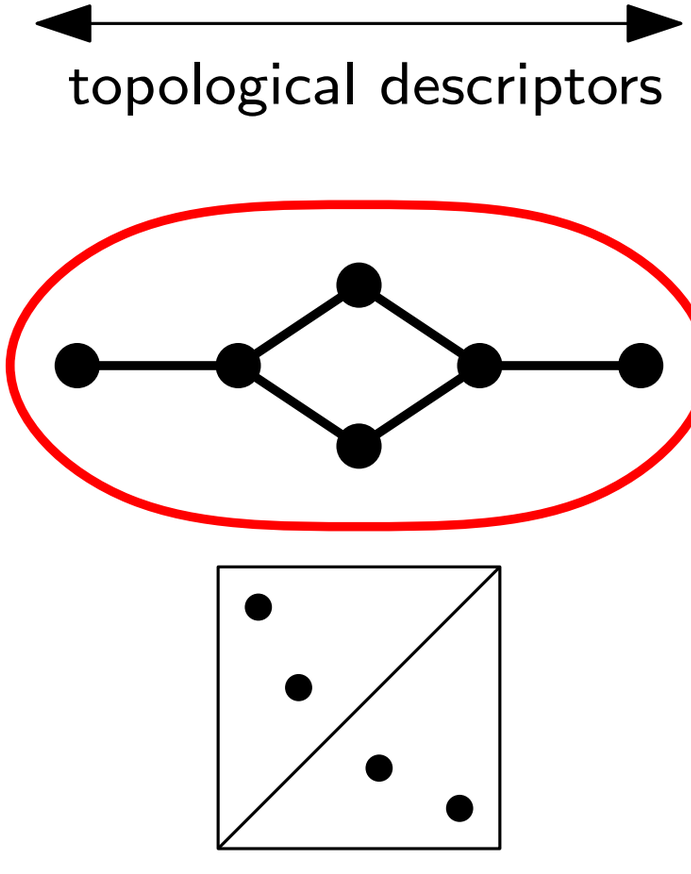
Why is topology interesting for data analysis?

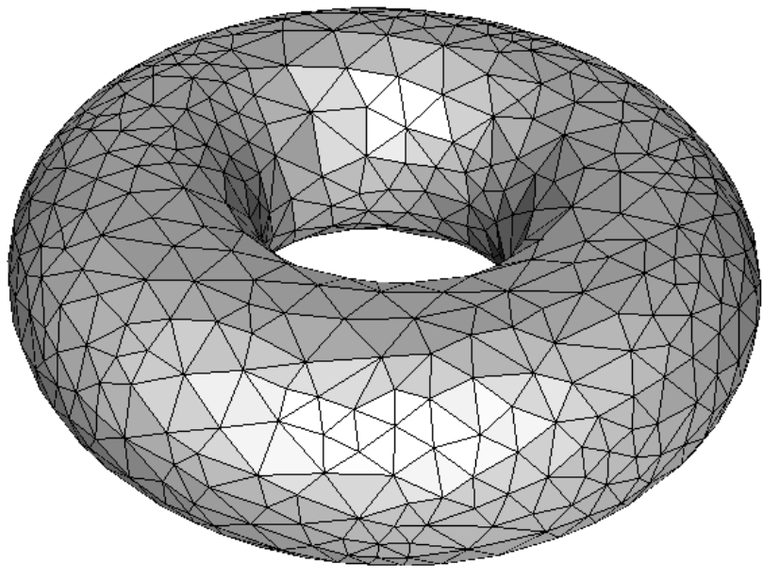
$\longrightarrow$ multiscale
$\longrightarrow$ compact

$\longrightarrow$ complementary to other descriptors
$\longrightarrow$ stable with respect to (small) perturbations
$\longrightarrow$ invariant under coordinate changes/rigid transforms



topological space

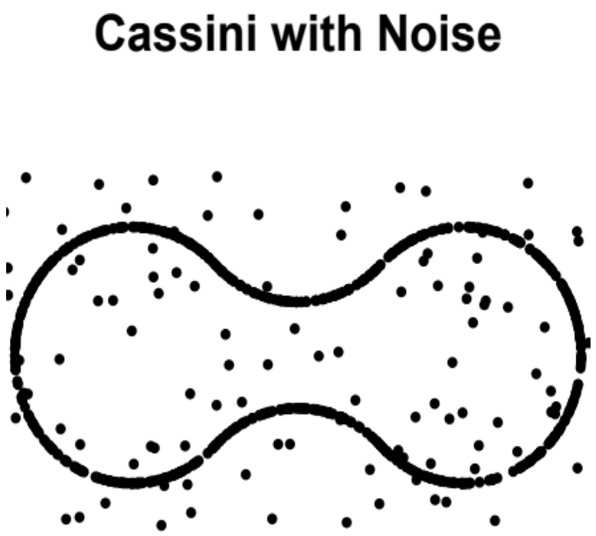


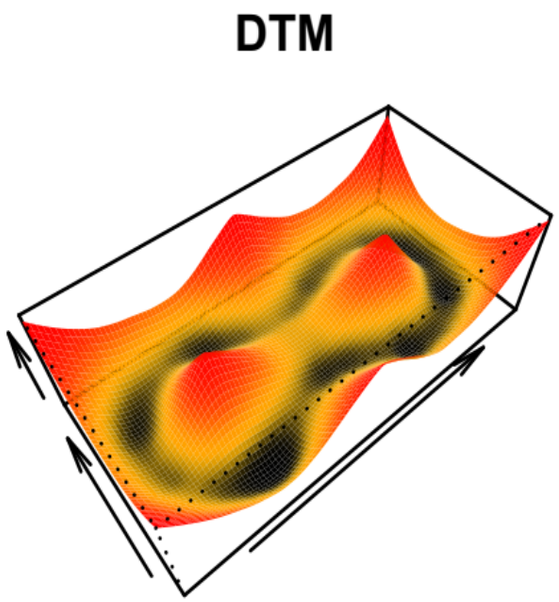


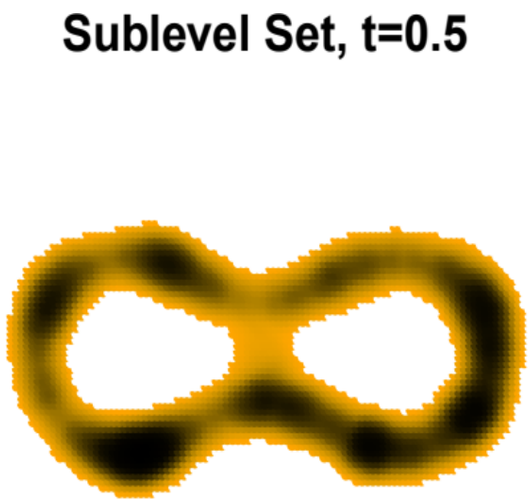
point cloud
triangulation

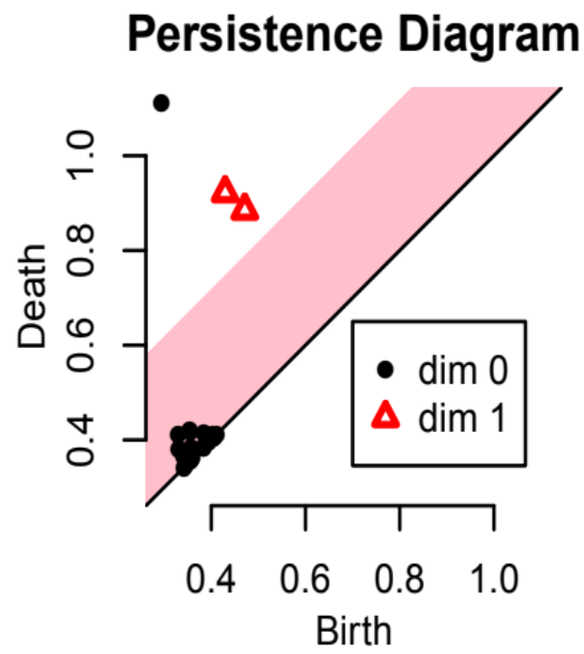
Topological Data Analysis

For **exploratory analysis**, visualization



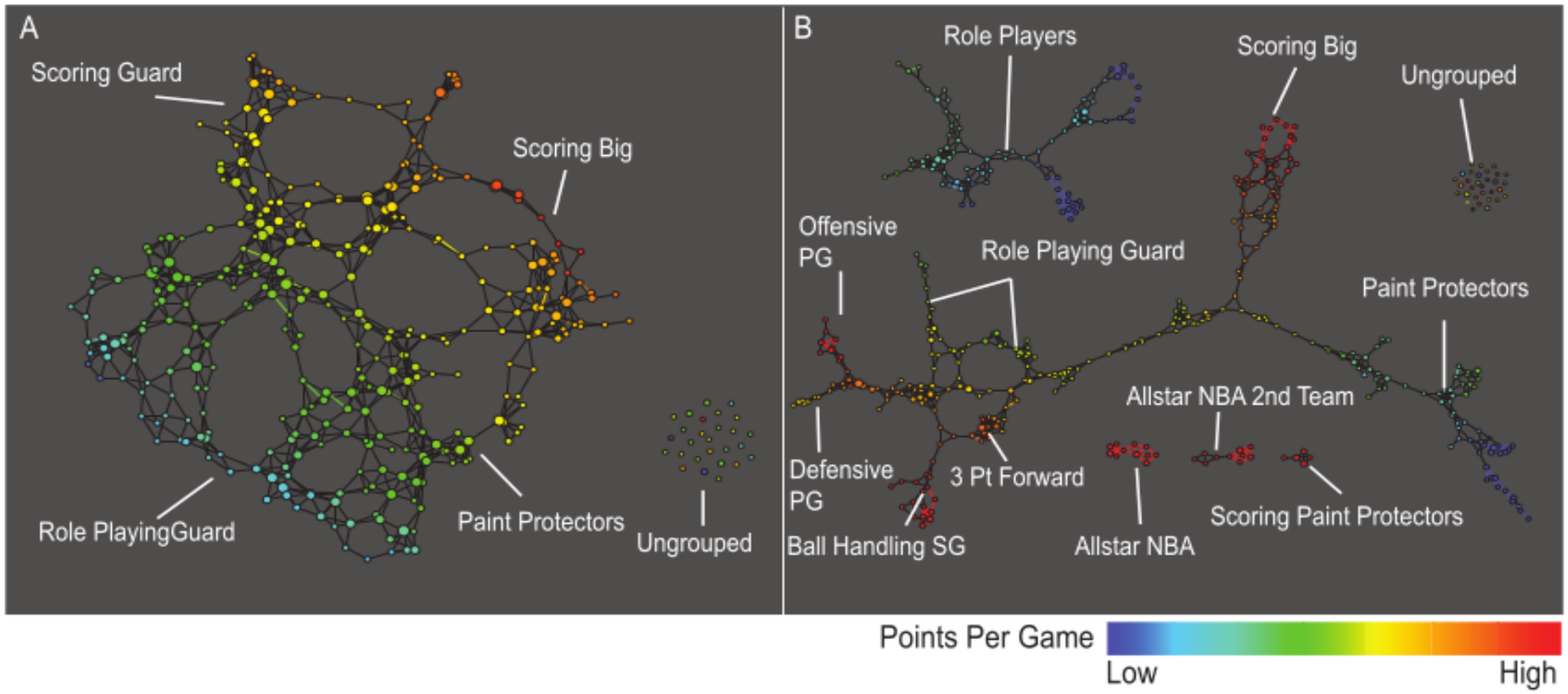






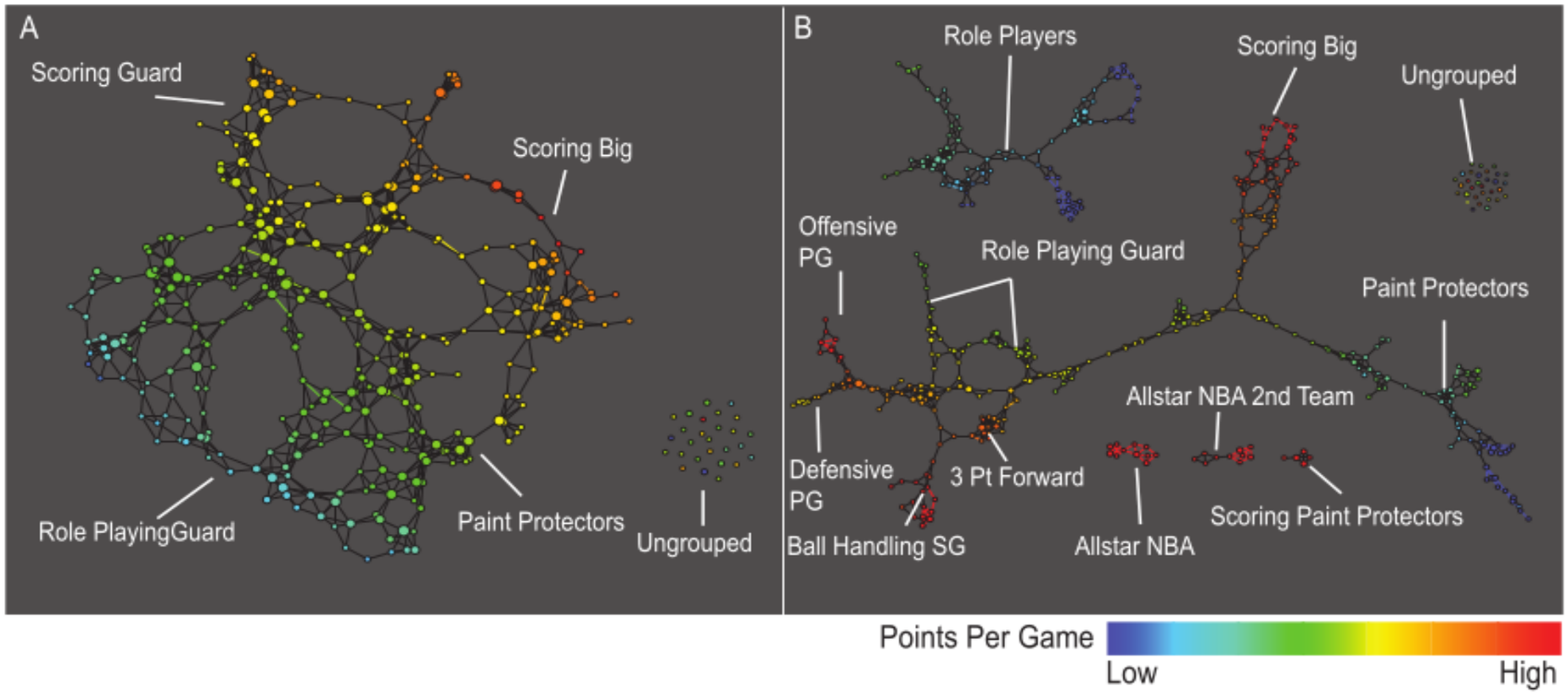
Topological Data Analysis

For **exploratory analysis**, visualization

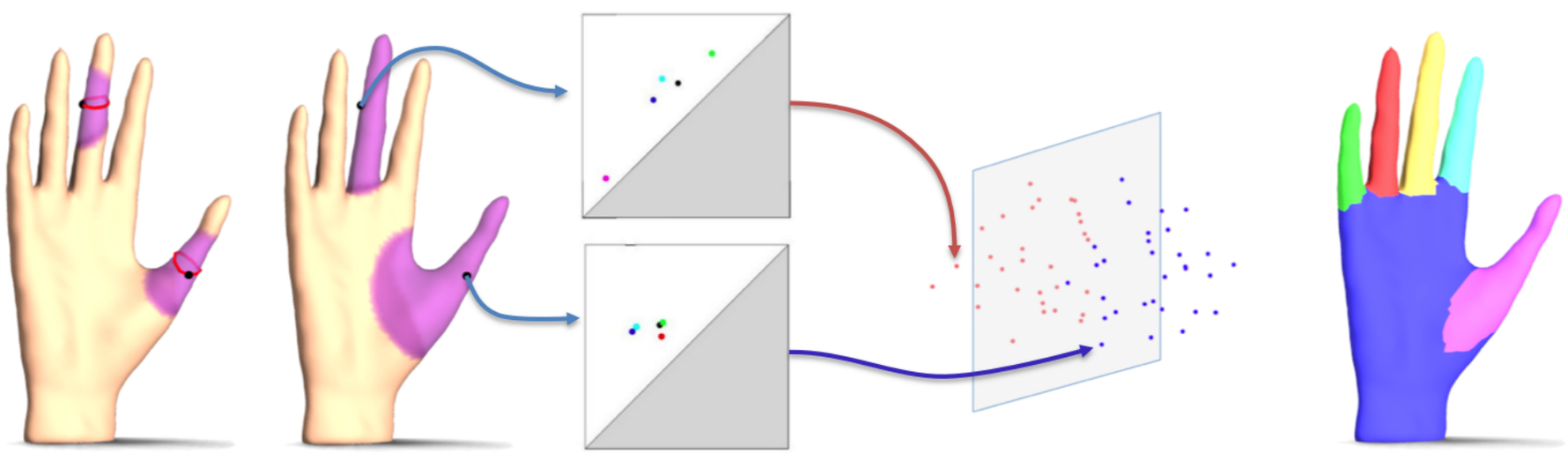


Topological Data Analysis

For **exploratory analysis**, visualization

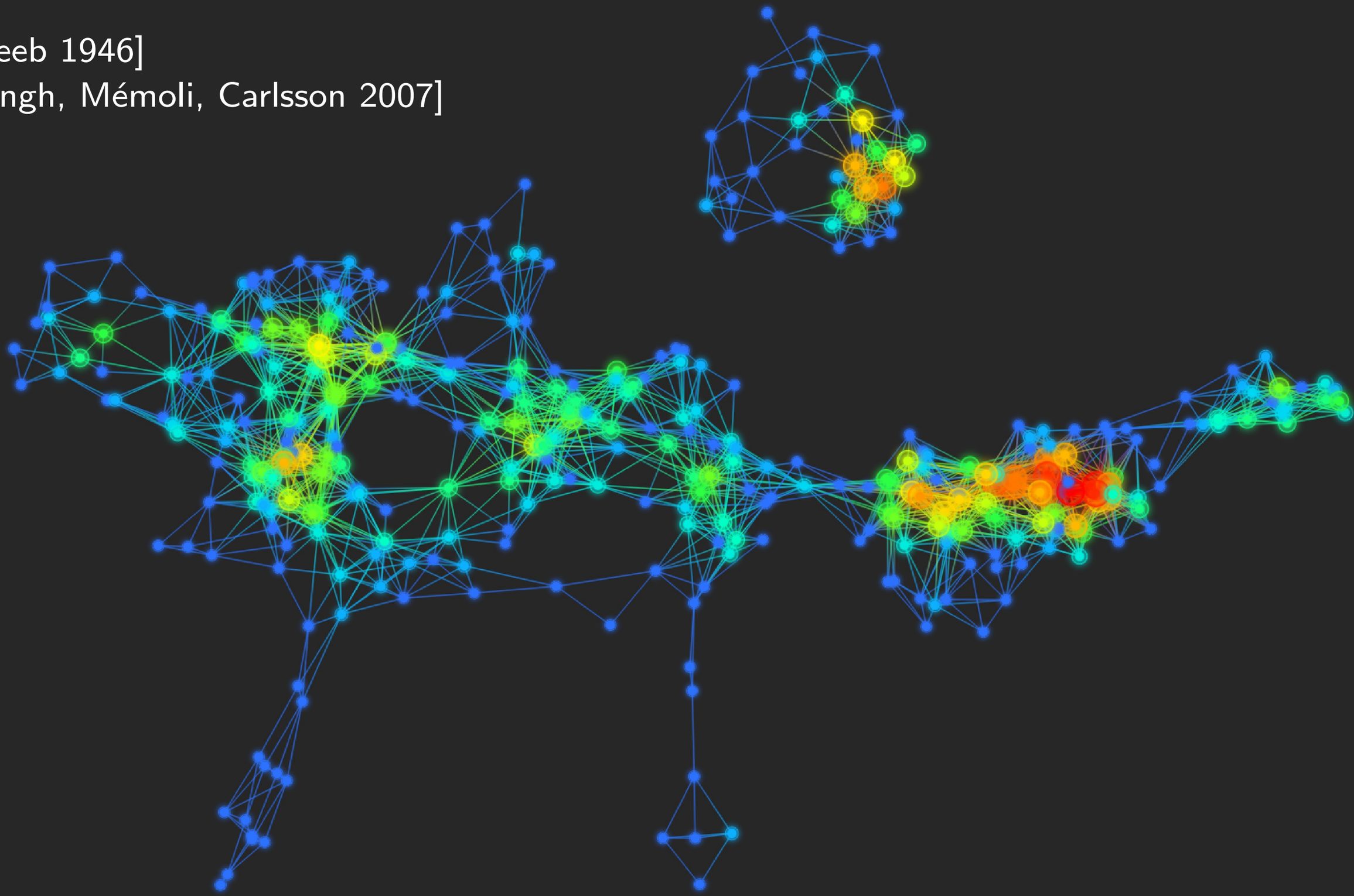


For **feature extraction** and **statistical learning**



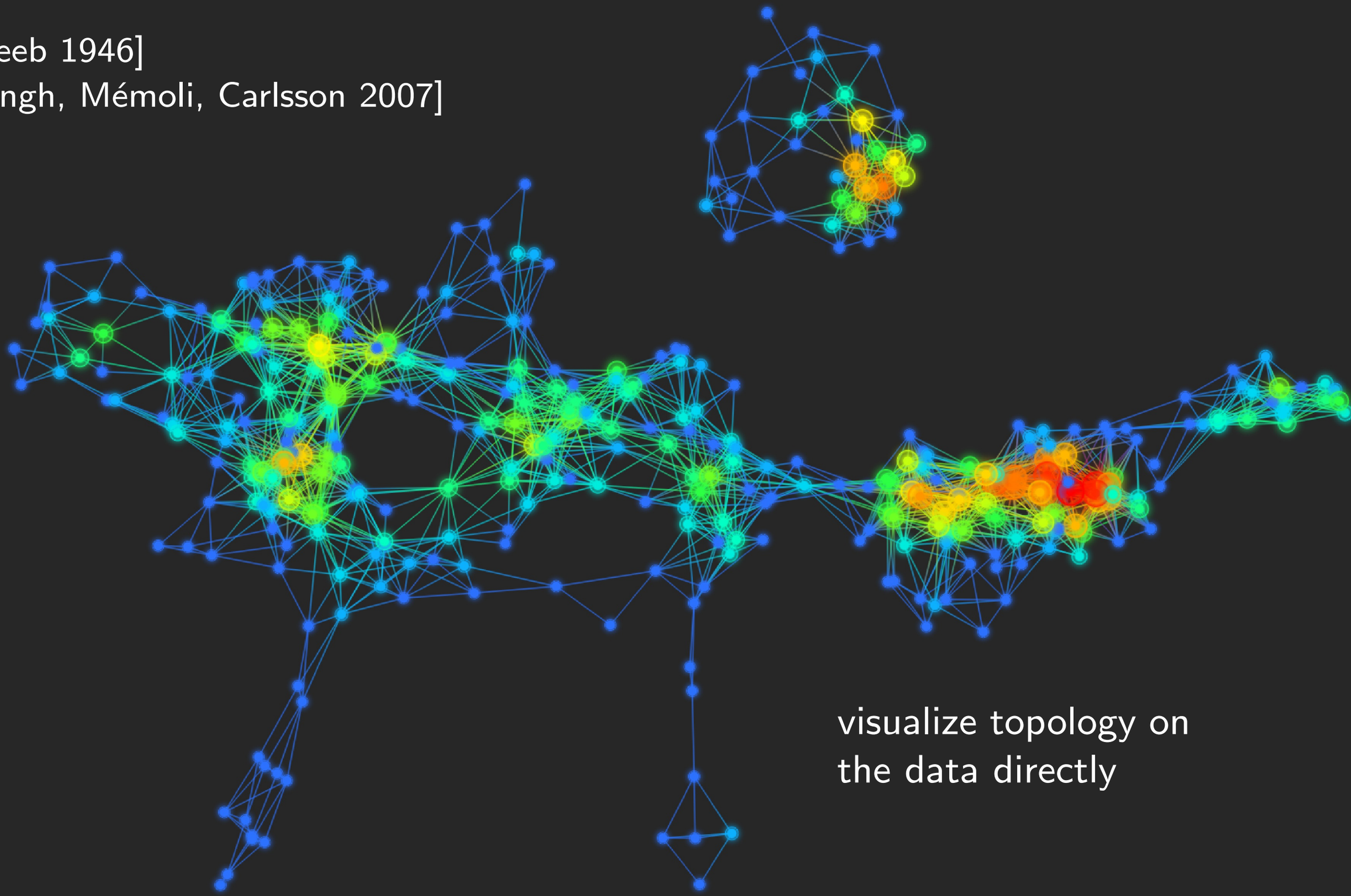
Reeb Graphs and Mapper

[Reeb 1946]
[Singh, Mémoli, Carlsson 2007]



Reeb Graphs and Mapper

[Reeb 1946]
[Singh, Mémoli, Carlsson 2007]



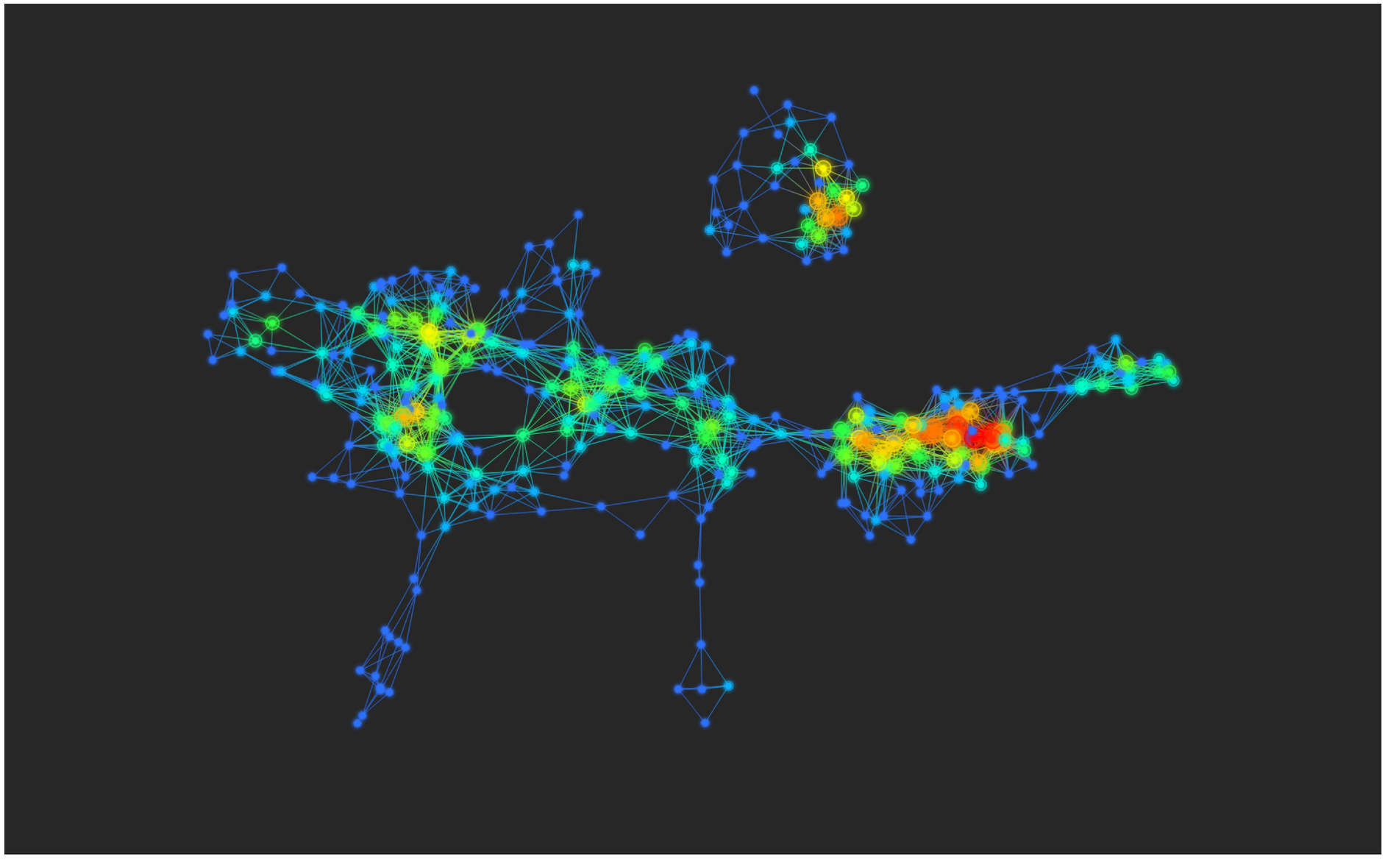
visualize topology on
the data directly

Applications

$\longrightarrow$ visualization

$\longrightarrow$ clustering

$\longrightarrow$ feature selection



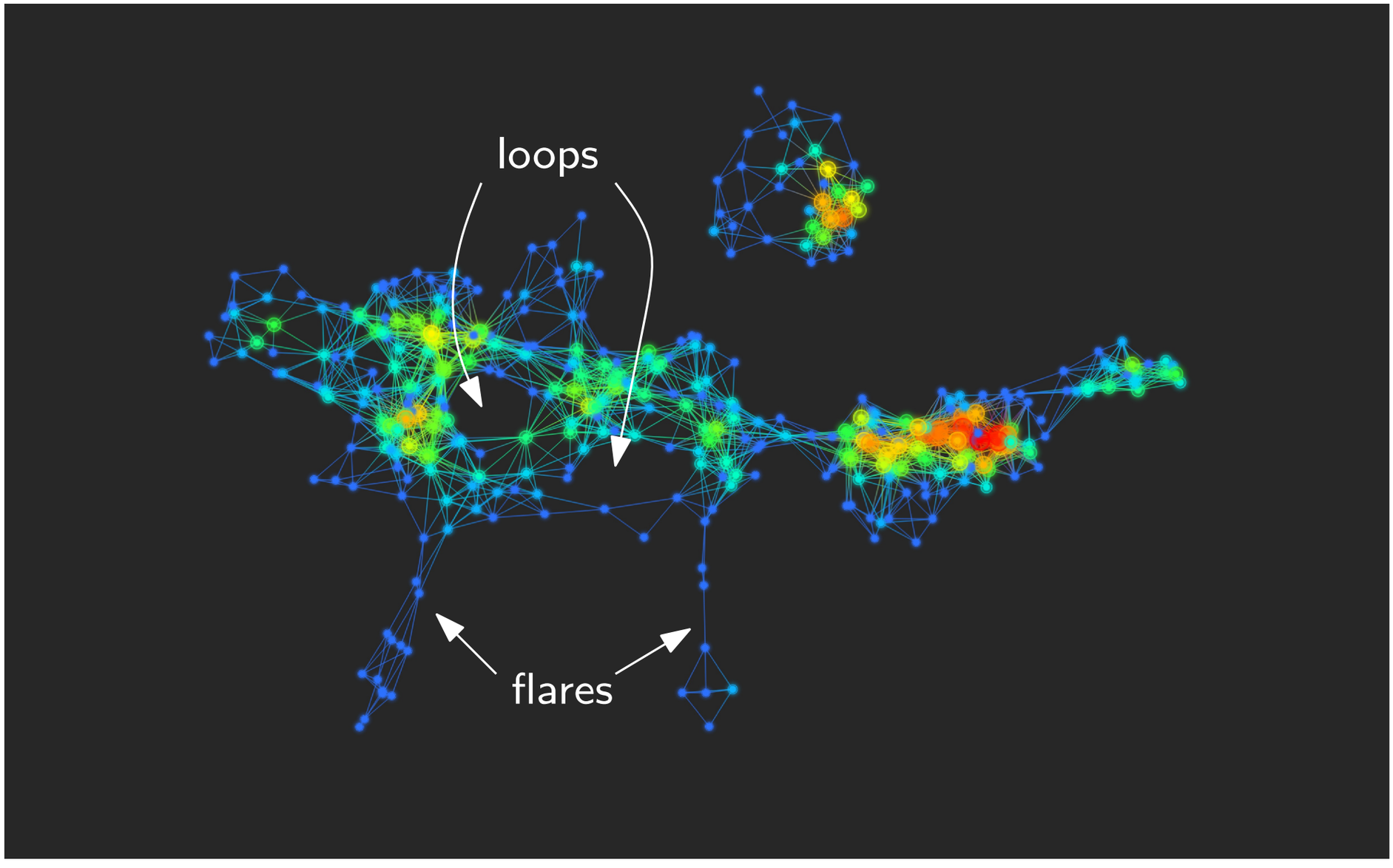
Applications

$\longrightarrow$ visualization

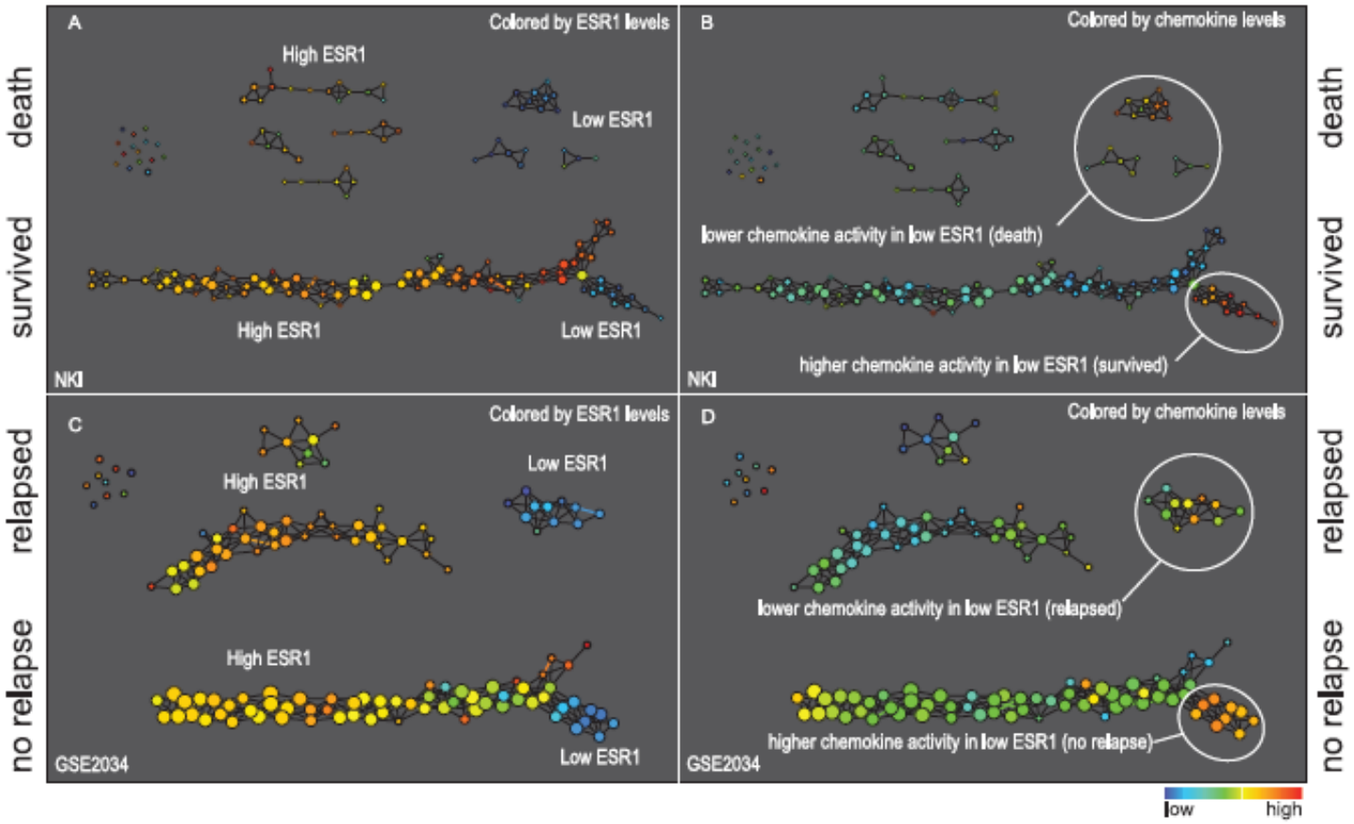
$\longrightarrow$ clustering

$\longrightarrow$ feature selection

Principle: identify statistically relevant sub-populations through patterns (flares, loops)

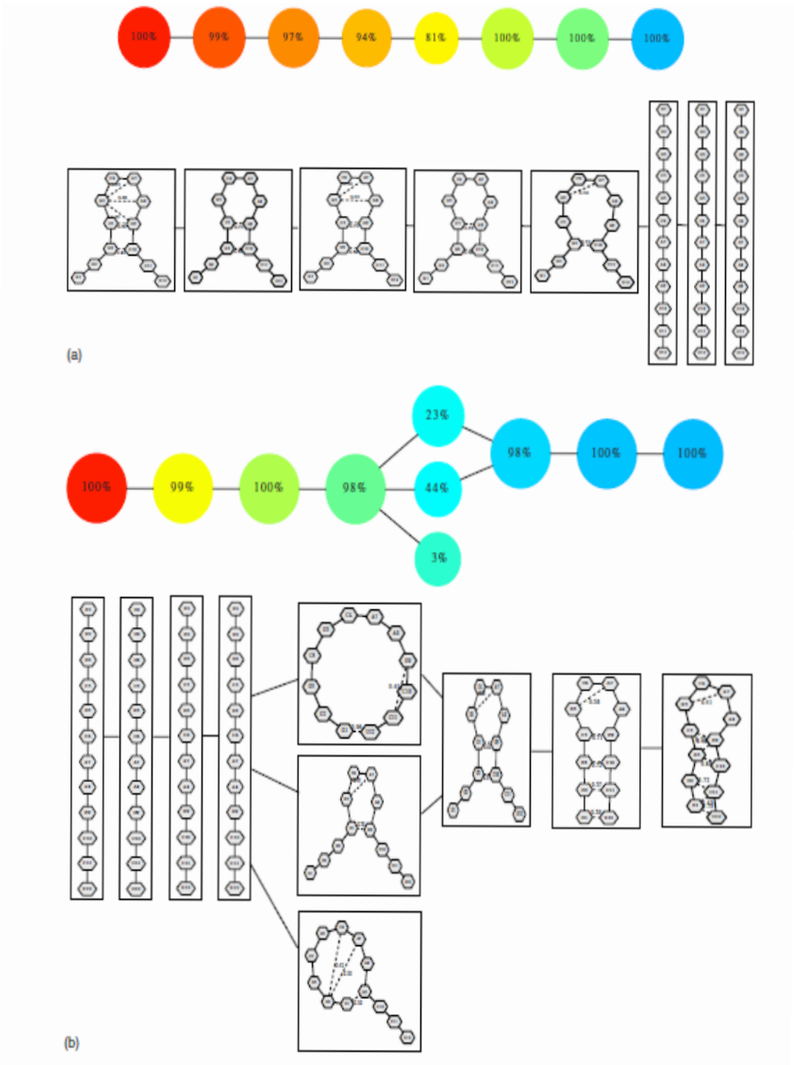


Applications



breast cancer subtype identification

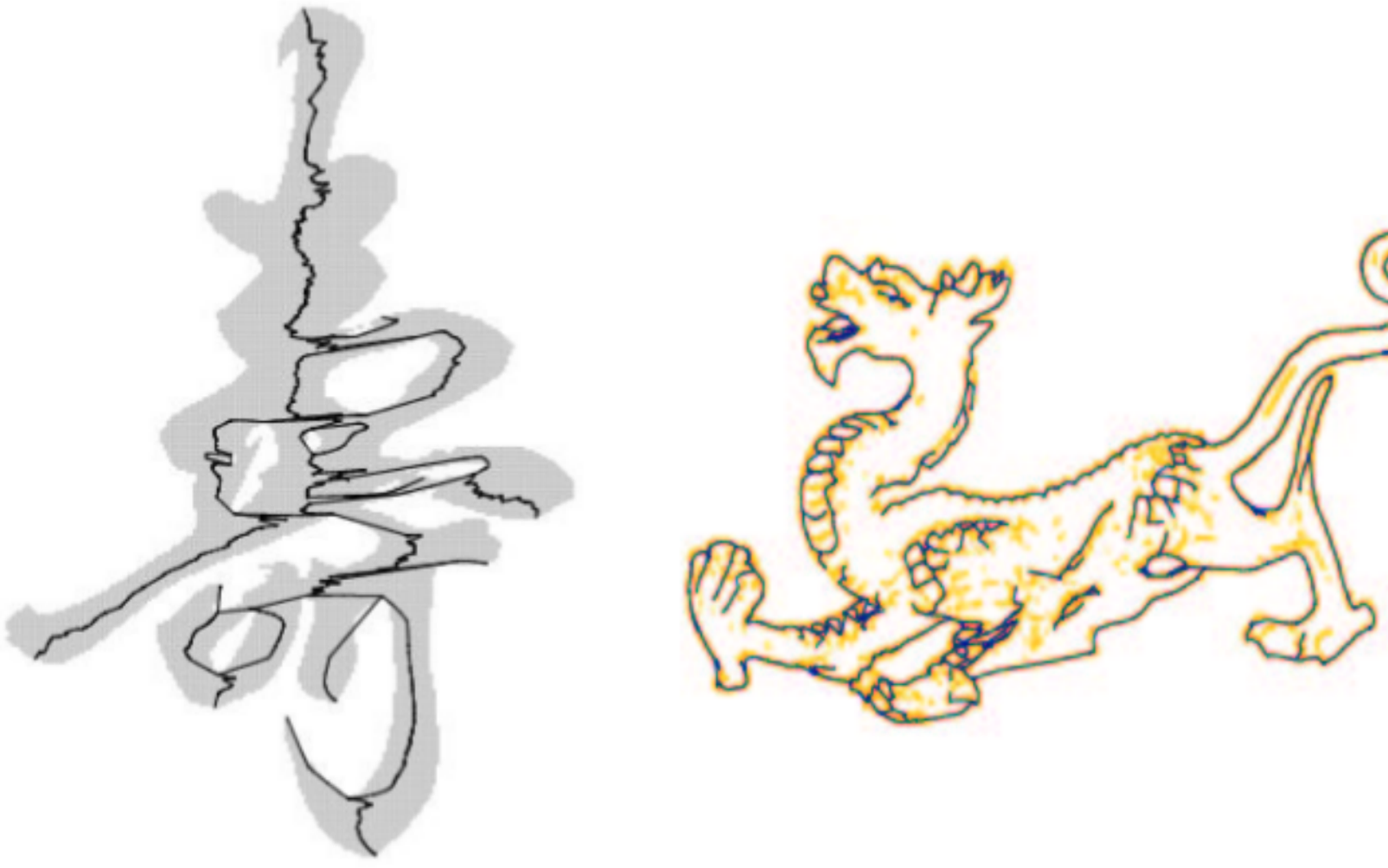
[Nicolau et al. 2011]



protein folding pathways

[Yao et al. 2009]

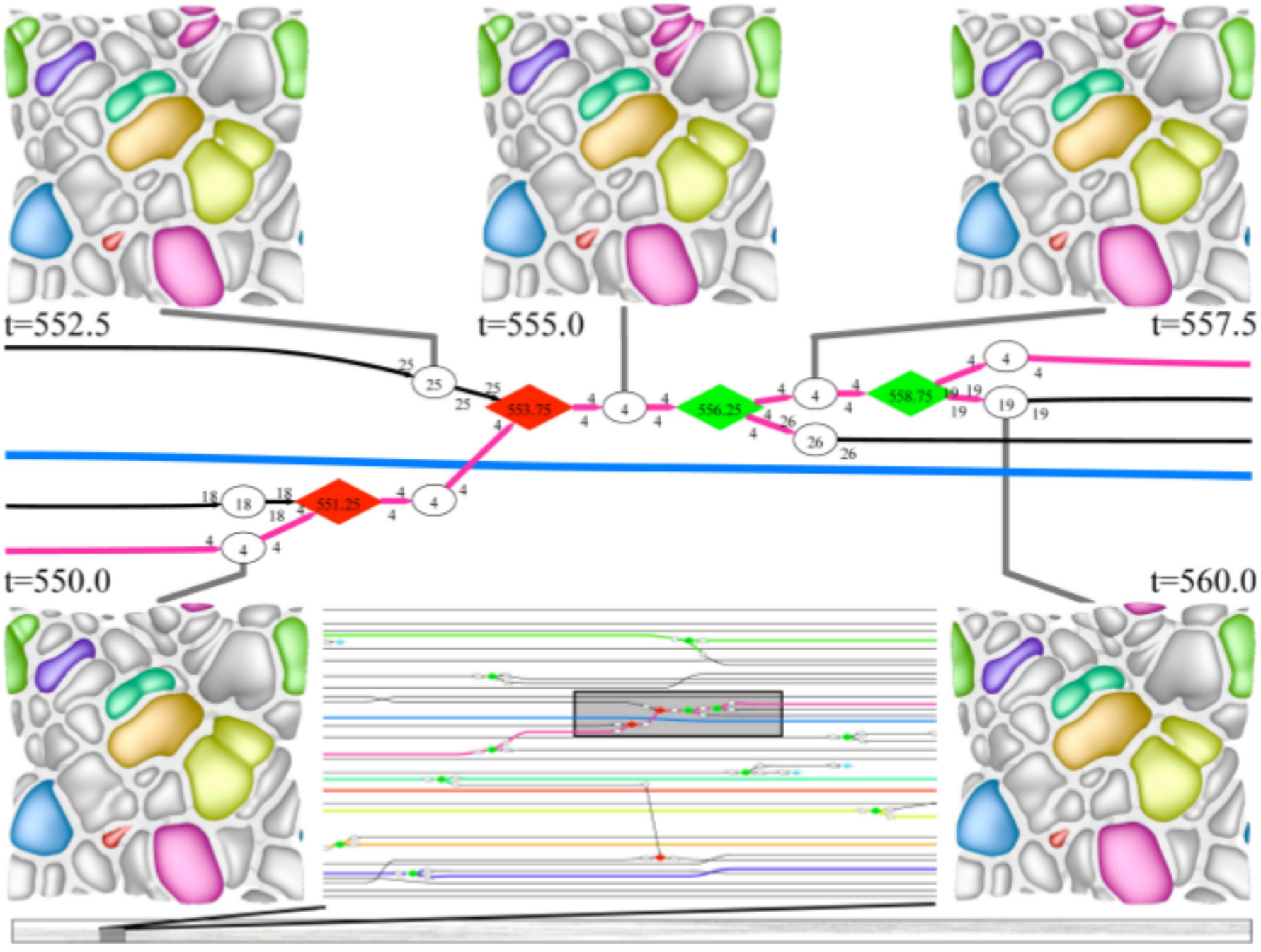
Applications



Data Skeletonization

[Ge et al. 2011]

Applications



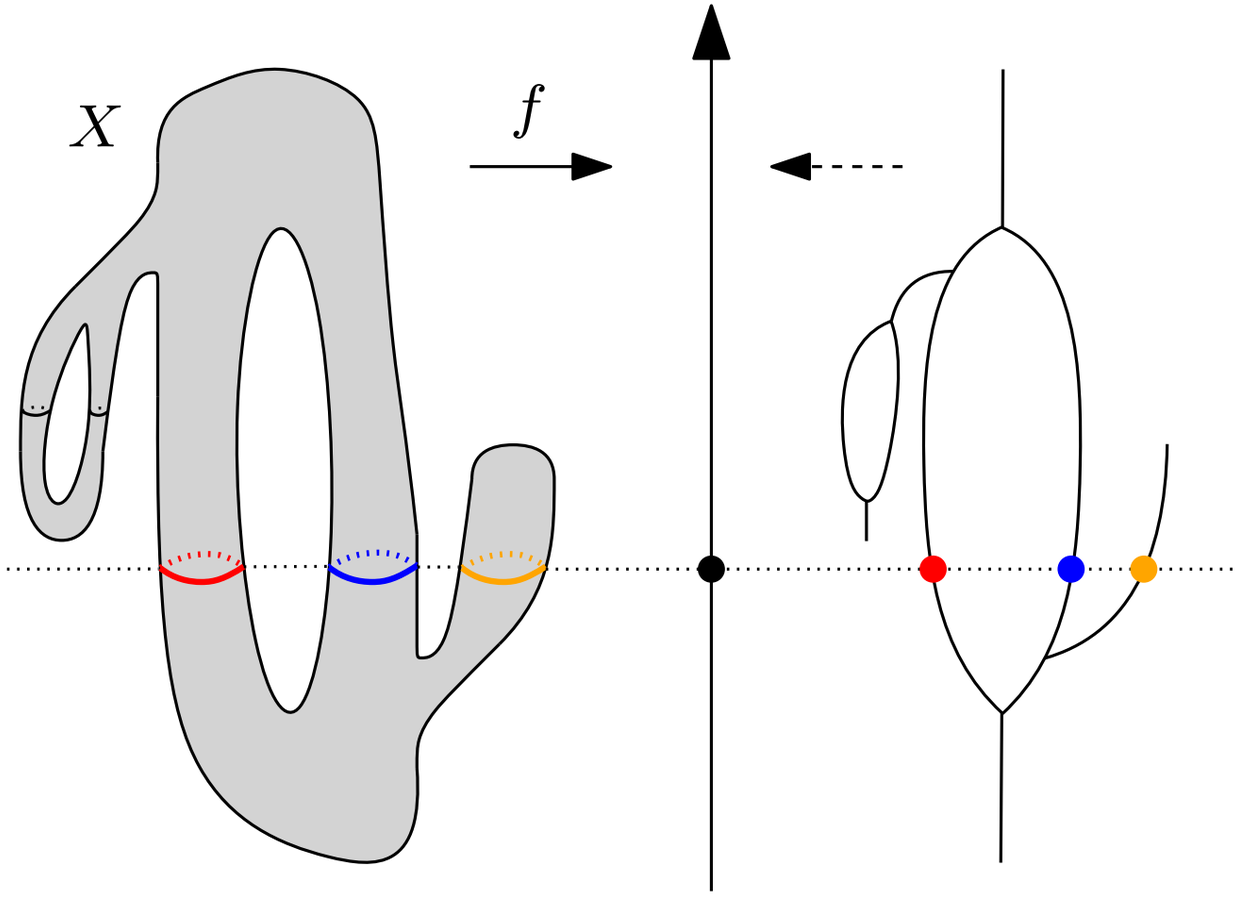
Burning regions of lean hydrogen flame over time

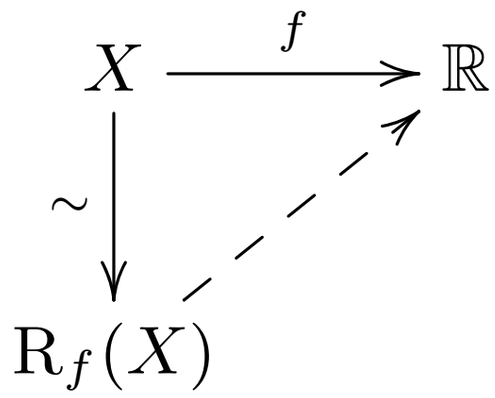
[Weber et al. 2011]

Reeb Graphs

$$x \sim y \iff [\ f(x) = f(y) \text{ and } x, y \text{ belong to same cc of } f^{-1}(f(x))\ ]$$

Def: $\mathrm{R}_f(X) = X/\sim$





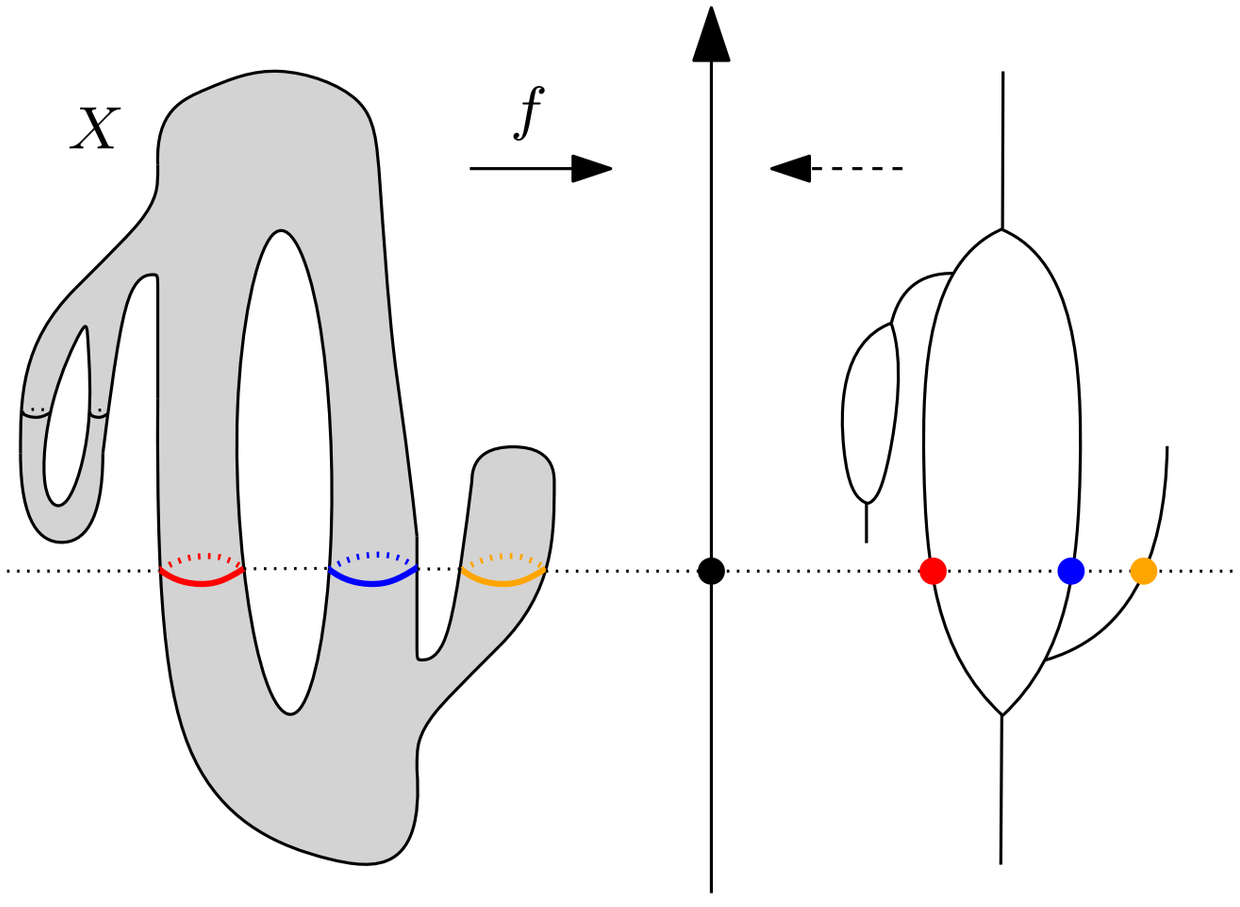
Prop: $\mathrm{R}_f(X)$ is a graph if (X, f) is of **Morse type**

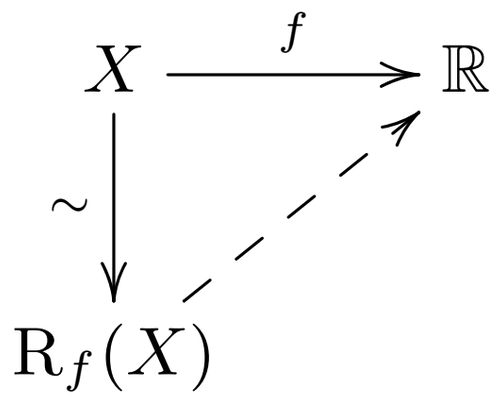
Reeb Graphs

$$x \sim y \iff [\ f(x) = f(y) \text{ and } x, y \text{ belong to same cc of } f^{-1}(f(x))\ ]$$

Def: $\mathrm{R}_f(X) = X/\sim$

Caveat: computation from point cloud is difficult





Prop: $\mathrm{R}_f(X)$ is a graph if (X, f) is of **Morse type**

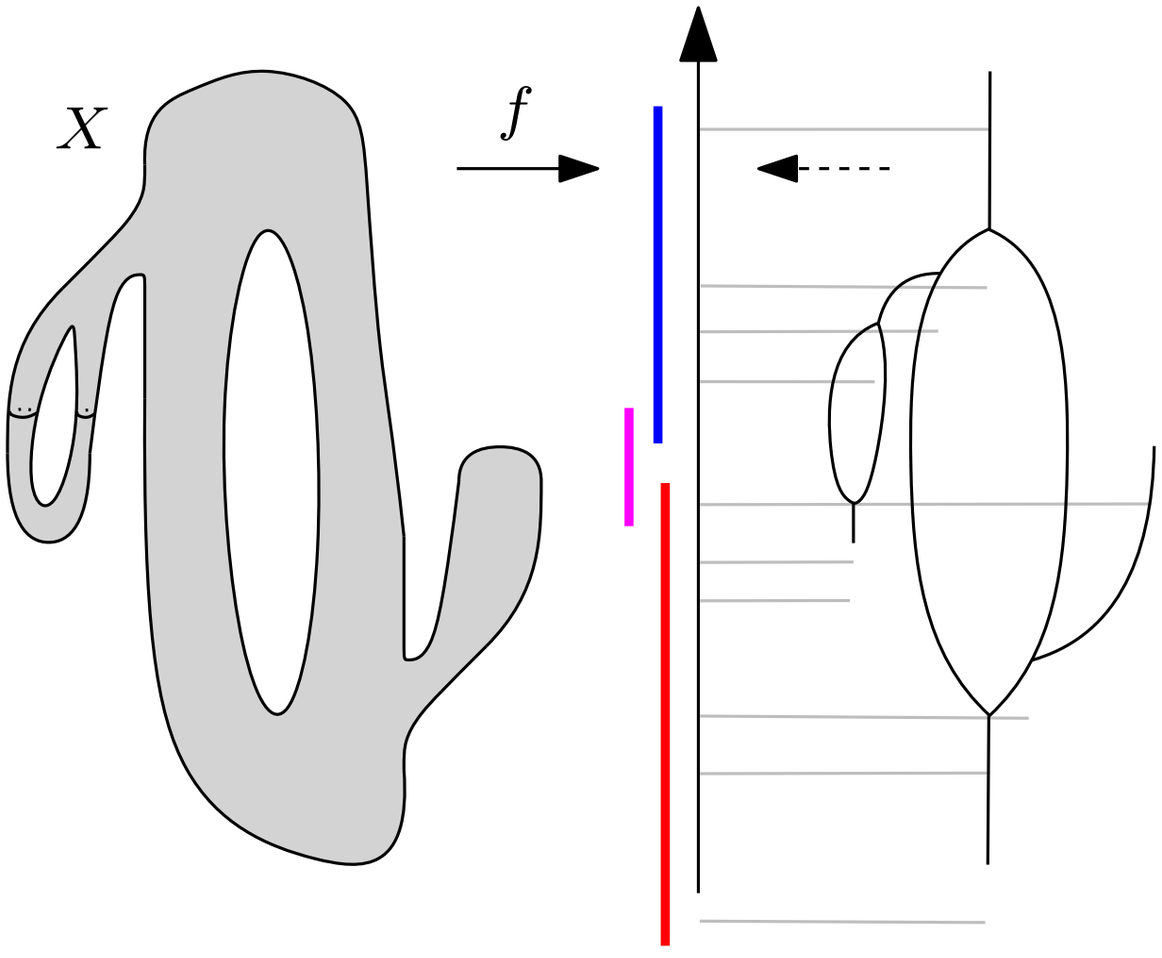
Reeb Graphs

$$x \sim y \iff [\ f(x) = f(y) \text{ and } x, y \text{ belong to same cc of } f^{-1}(f(x))\ ]$$

Def: $\mathrm{R}_f(X) = X/\sim$

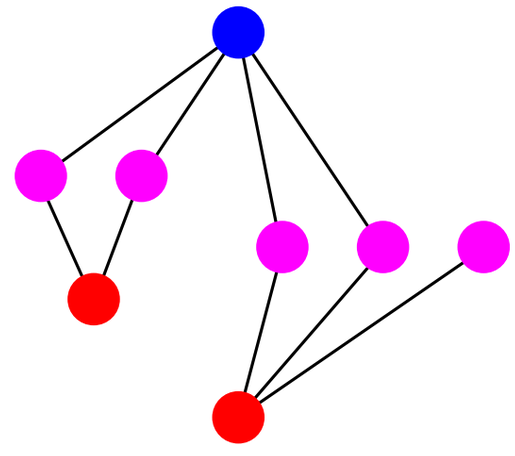
Caveat: computation from point cloud is difficult

$\rightarrow$ Proxy: **Mapper**

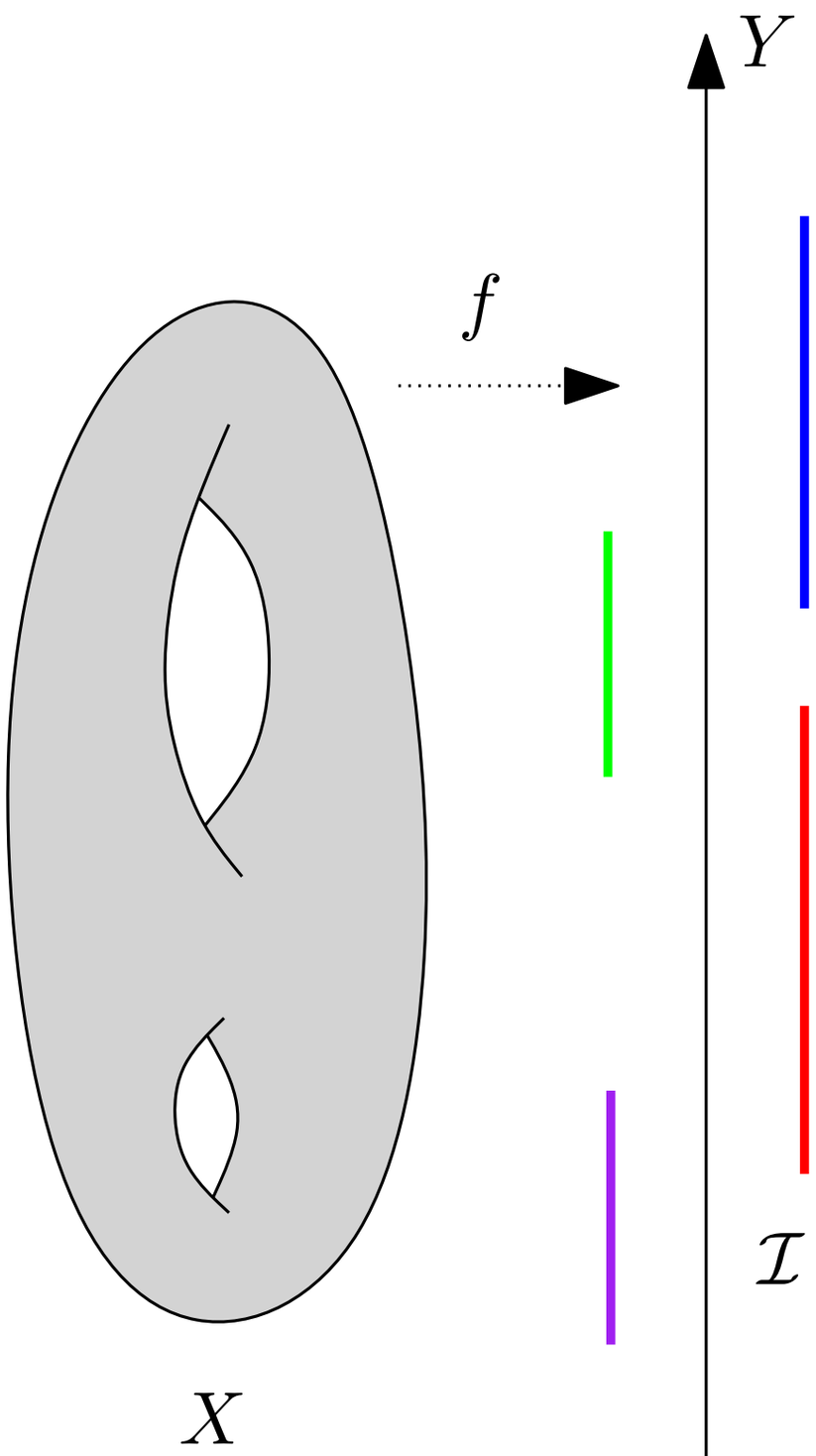


Pixelized Reeb graph

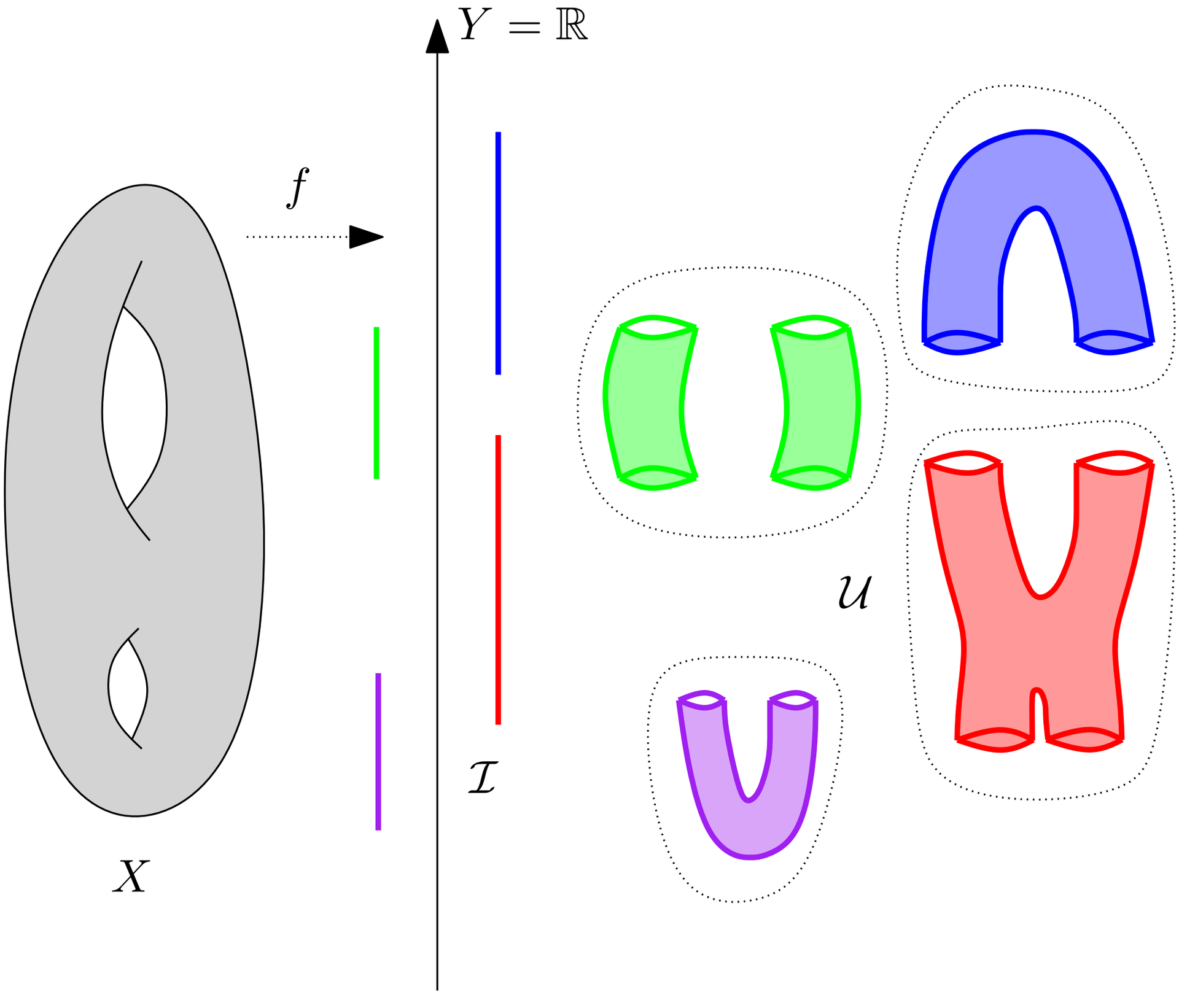
Singleton $\rightarrow$ interval: $f^{-1}(I)$



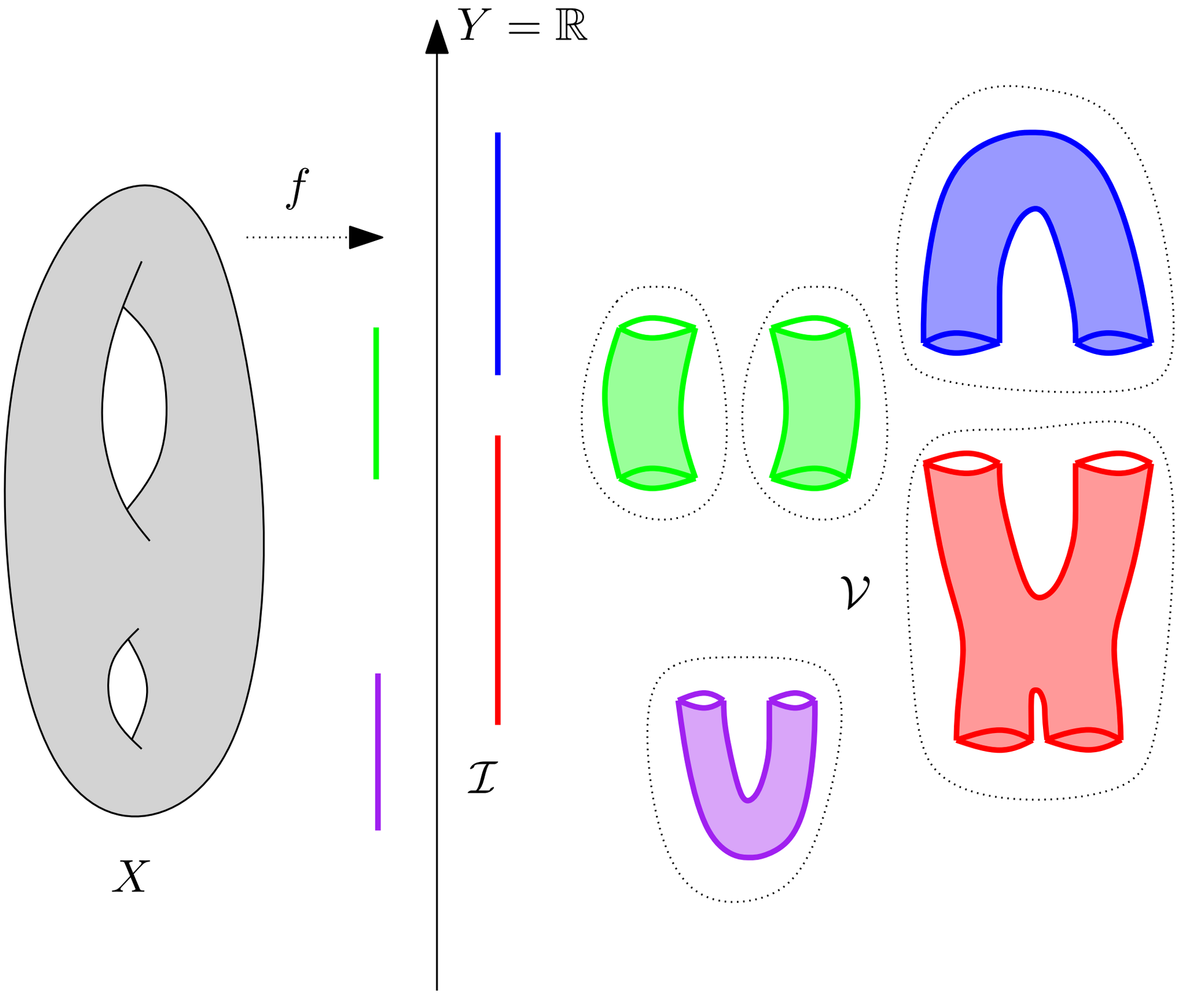
Mapper (continuous setting)



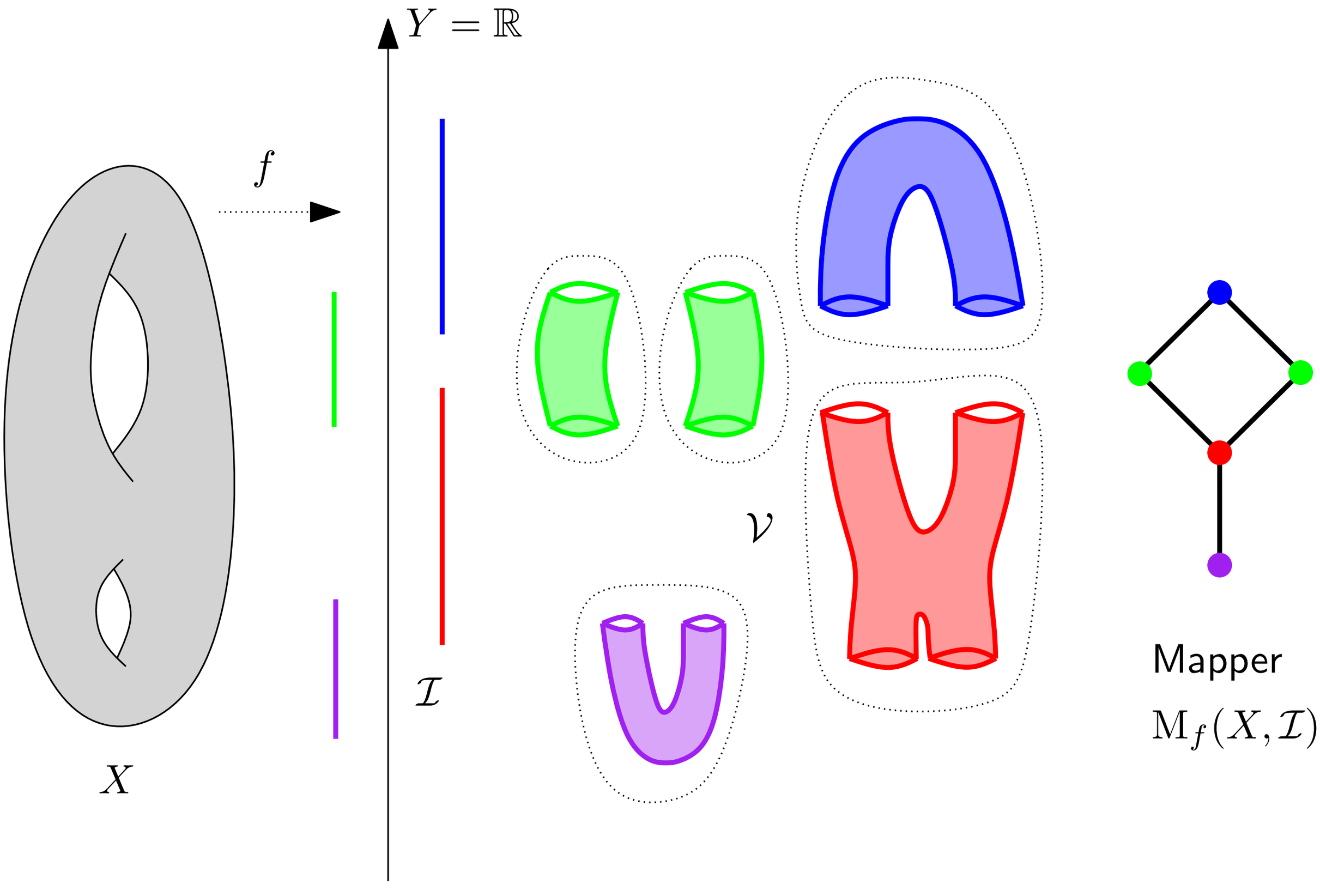
Mapper (continuous setting)



Mapper (continuous setting)



Mapper (continuous setting)



Mapper (continuous setting)

Input:

- topological space X
- continuous function $f : X \to \mathbb{R}$
- cover $\mathcal{I}$ of $\mathrm{im}(f)$ by open intervals: $\mathrm{im}(f) \subseteq \bigcup_{I \in \mathcal{I}} I$

Method:

- Compute *pullback cover* $\mathcal{U}$ of X: $\mathcal{U} = \{f^{-1}(I)\}_{I \in \mathcal{I}}$
- Refine $\mathcal{U}$ by separating the connected components
- The Mapper is the *nerve* of $\mathcal{V}$:
  - 1 vertex per element $V \in \mathcal{V}$
  - 1 edge per intersection $V \cap V' \neq \emptyset$, $V, V' \in \mathcal{V}$
  - 1 k-simplex per $(k+1)$-fold intersection $\bigcap_{i=0}^{k} V_i \neq \emptyset$, $V_0, \cdots, V_k \in \mathcal{V}$

Mapper (discrete setting)

Input:

- point cloud $P \subseteq X$ with metric d_P
- continuous function $f : P \to \mathbb{R}$
- cover $\mathcal{I}$ of $\mathrm{im}(f)$ by open intervals: $\mathrm{im} f \subseteq \bigcup_{I \in \mathcal{I}} I$

Method:

• Compute *pullback cover* $\mathcal{U}$ of P: $\mathcal{U} = \{f^{-1}(I)\}_{I \in \mathcal{I}}$

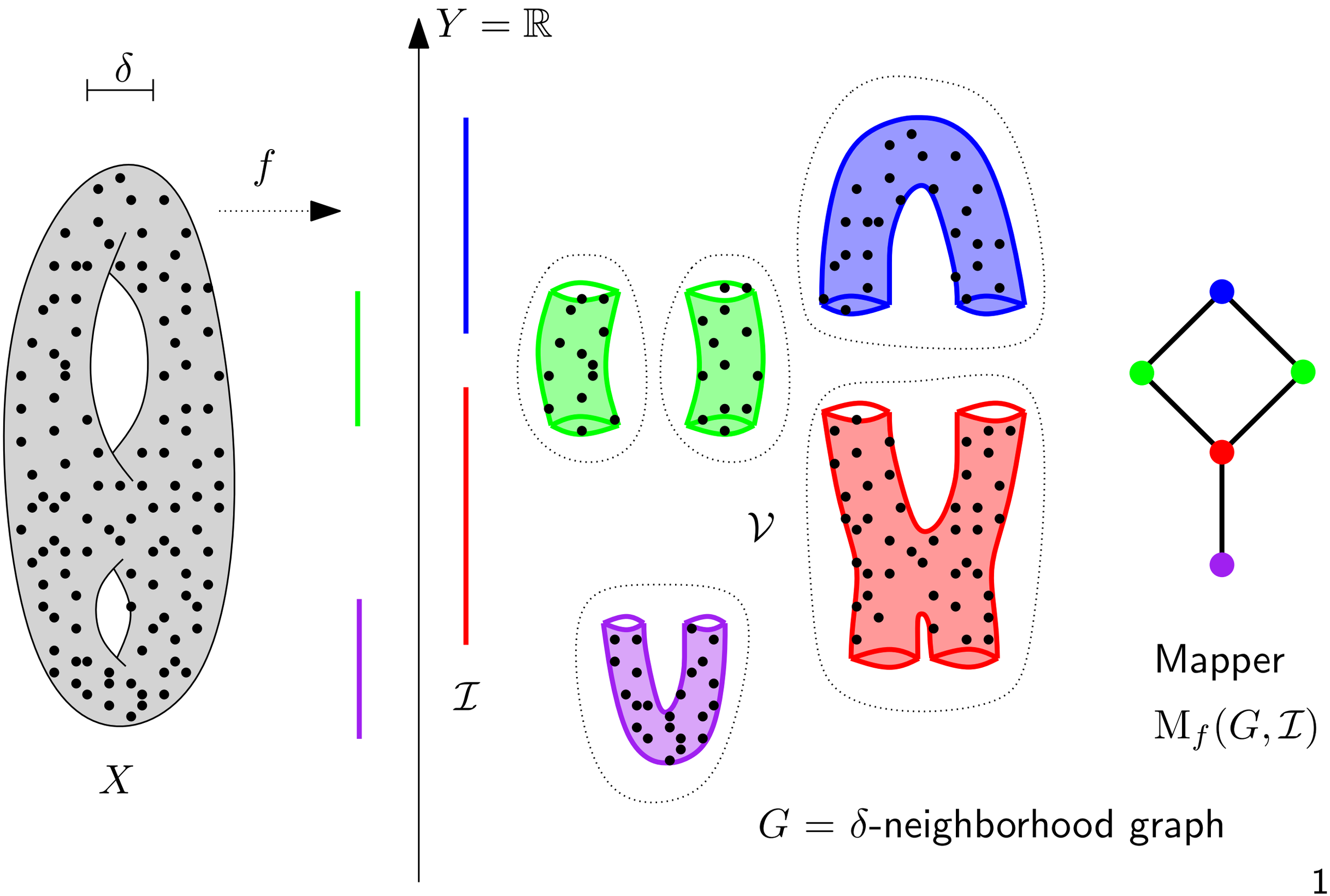
• Refine $\mathcal{U}$ by separating each of its elements into its various connected components in $G \to$ connected cover $\mathcal{V}$

• The Mapper is the *nerve* of $\mathcal{V}$:

(intersections materialized by data points)

- 1 vertex per element $V \in \mathcal{V}$
- 1 edge per intersection $V \cap V' \neq \emptyset$, $V, V' \in \mathcal{V}$
- 1 k-simplex per $(k+1)$-fold intersection $\bigcap_{i=0}^{k} V_i \neq \emptyset$, $V_0, \cdots, V_k \in \mathcal{V}$

Mapper (discrete setting)



Parameters

- function $f : P \to \mathbb{R}$

lens or filter

- cover $\mathcal{I}$ of $\mathrm{im}(f)$ by open intervals

range scale

- neighborhood size δ

geometric scale

Parameters

- function $f : P \to \mathbb{R}$

lens or filter

- cover $\mathcal{I}$ of $\mathrm{im}(f)$ by open intervals

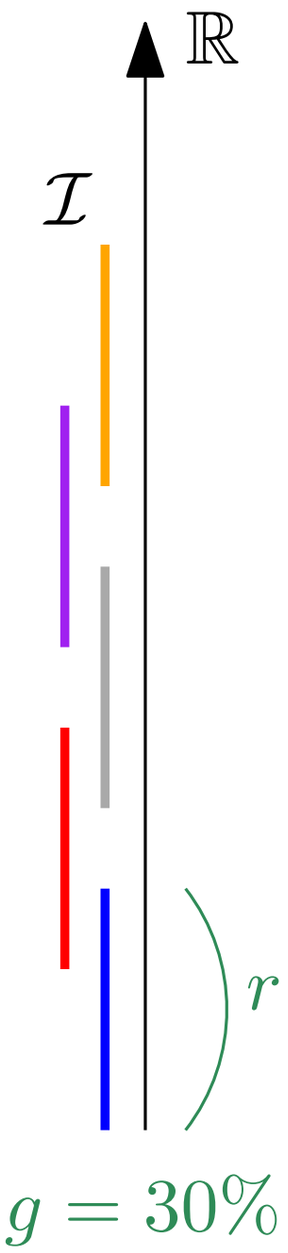
range scale

- neighborhood size δ

geometric scale

uniform cover $\mathcal{I}$:

- resolution / granularity: r (diameter of intervals)
- gain: g (percentage of overlap)

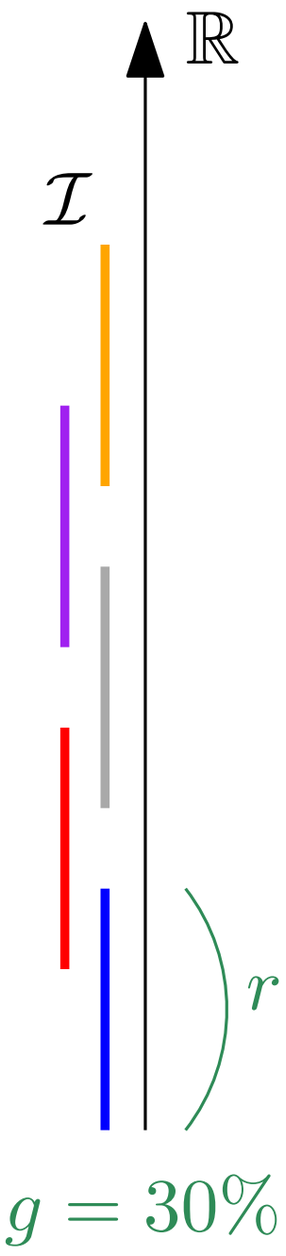


Parameters

- function $f : P \to \mathbb{R}$ — lens or filter
- cover $\mathcal{I}$ of $\mathrm{im}(f)$ by open intervals
- neighborhood size δ

geometric scale

range scale



uniform cover $\mathcal{I}$:

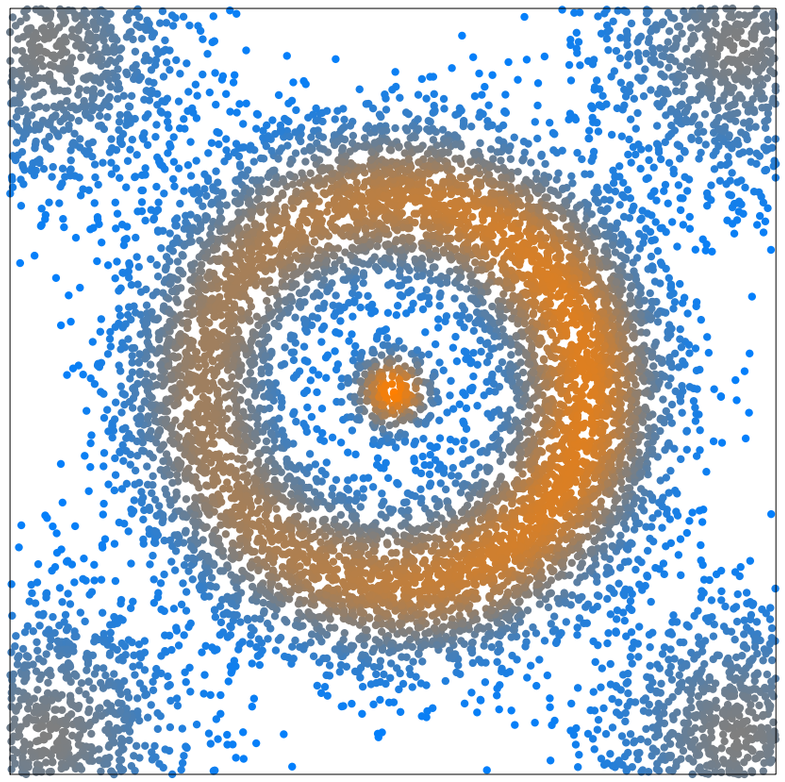
- resolution / granularity: r (diameter of intervals)
- gain: g (percentage of overlap)

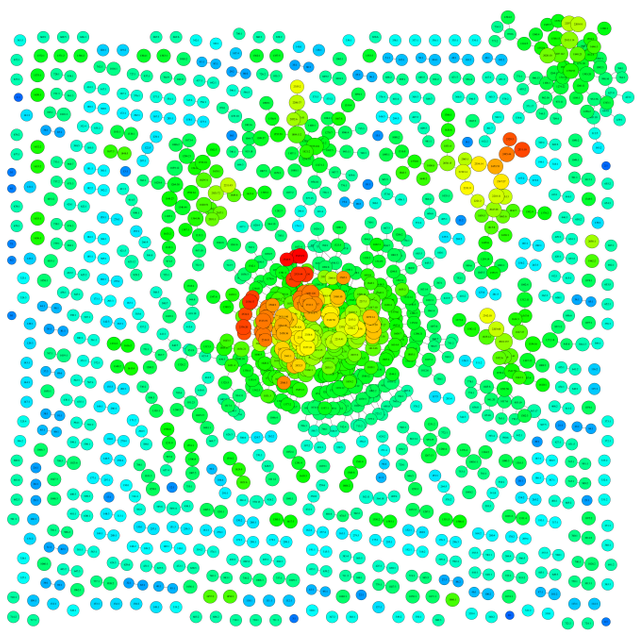
In practice: trial-and-error

Examples

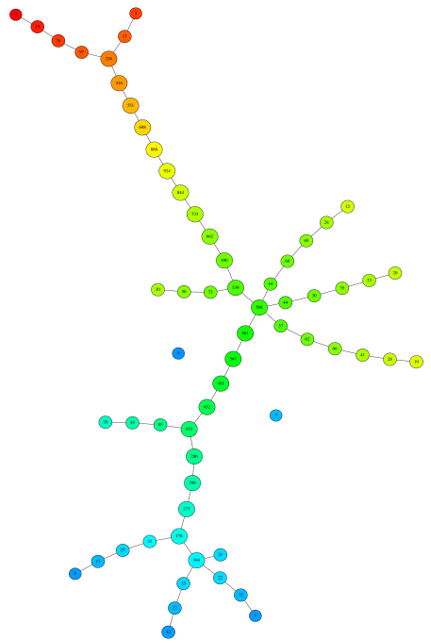
$\hat{f}$ = density estimator

$r = 0.3,\ g = 20\%$

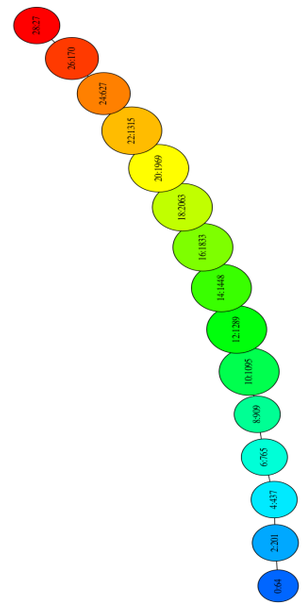




$\delta = 0.1\%$

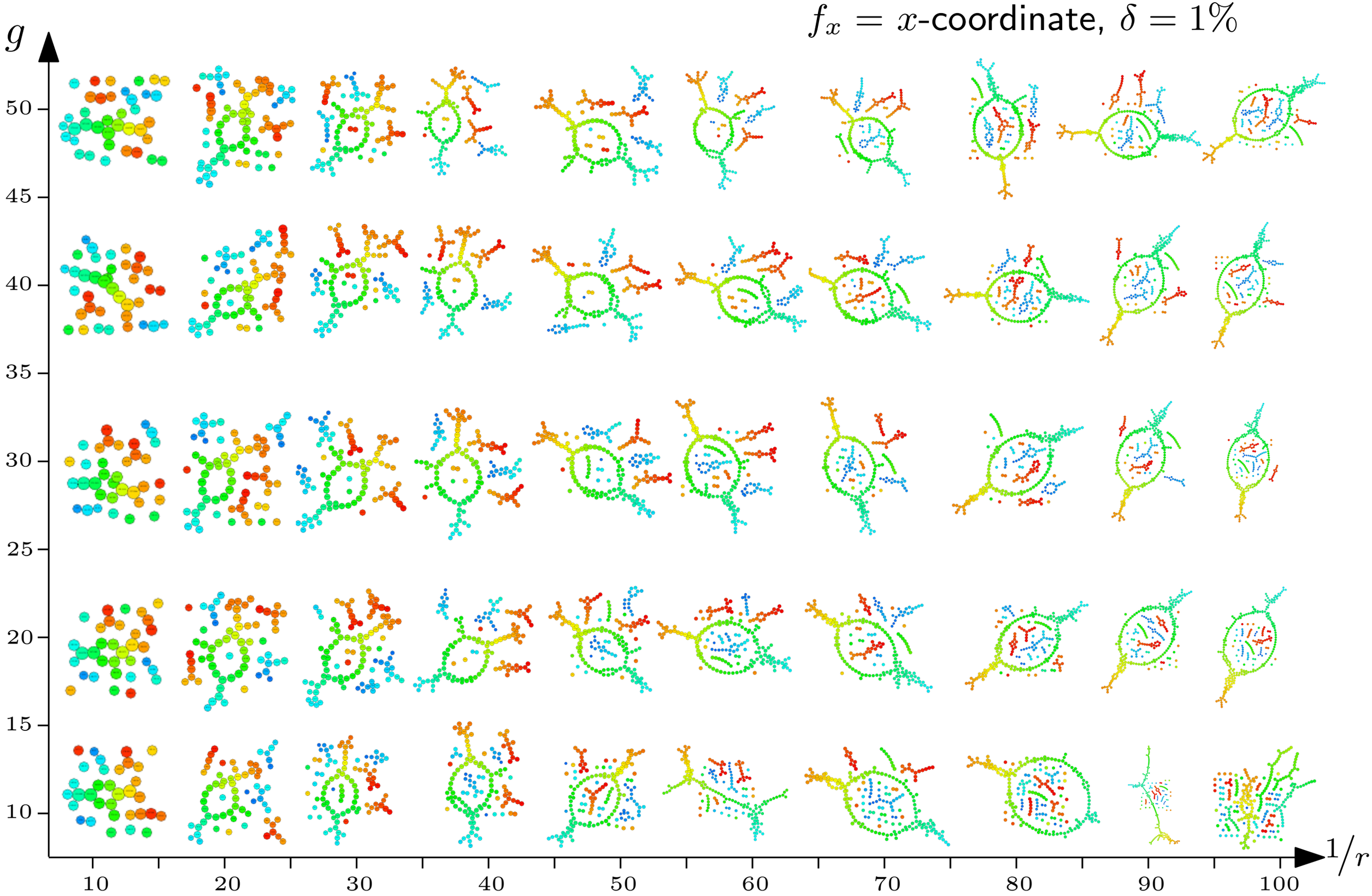


$\delta = 1\%$



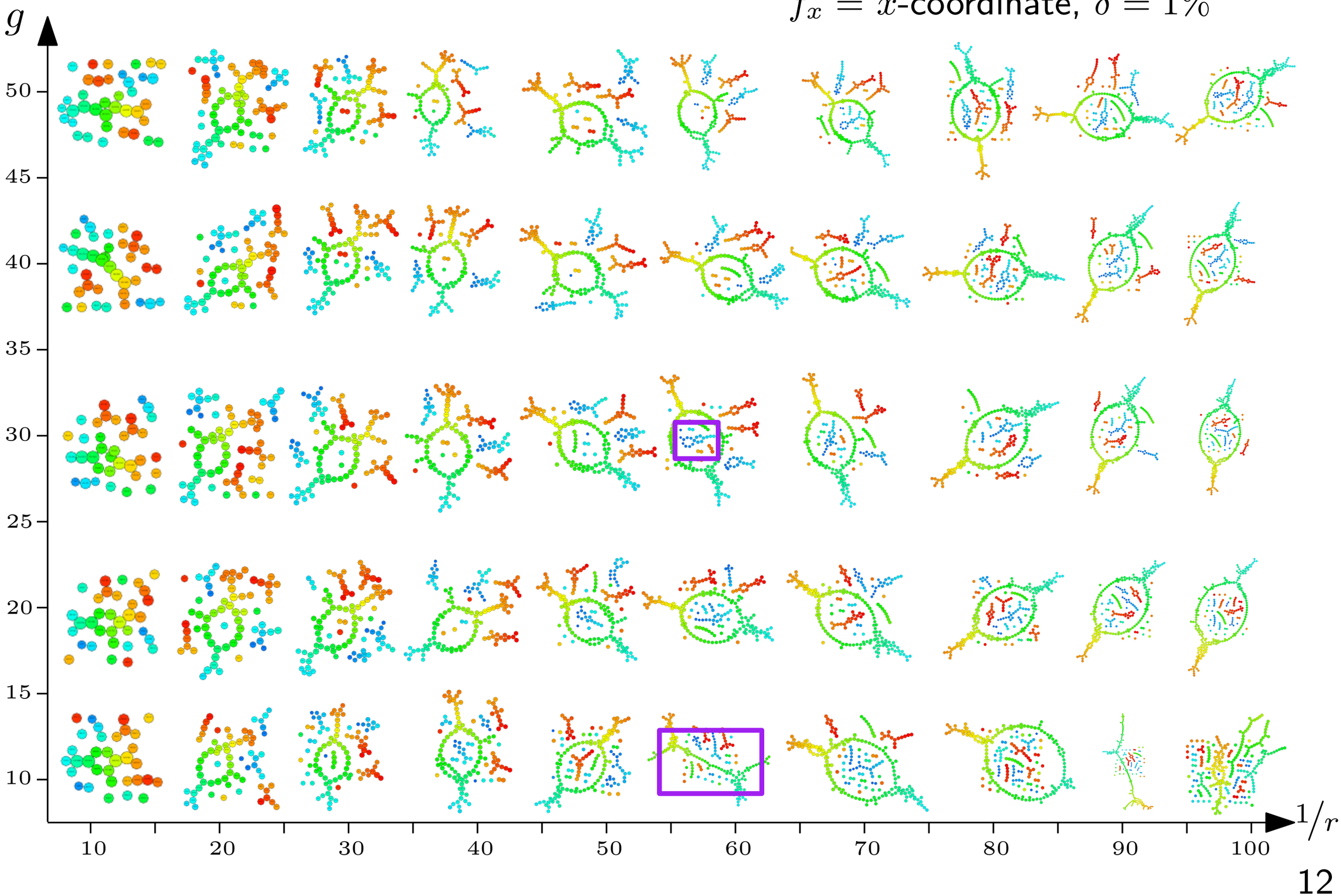
$\delta = 10\%$

Examples


$f_x = x$-coordinate, $\delta = 1\%$
g
50
45
40
35
30
25
20
15
10
$1/r$
10
20
30
40
50
60
70
80
90
100

Examples

$f_x = x$-coordinate, $\delta = 1\%$



Contributions

Structure of Mapper depending on r, g, δ [C., Oudot 2016-17]

Heuristics and Statistics for Mapper [C., Michel, Oudot 2017]

Local Equivalence of Mapper and PDs [C., Oudot 2017]

Machine Learning for Mapper (through PDs):

- Finite dimensional kernel [C., Ovsjanikov, Oudot 2015]
- Gaussian kernel [C., Cuturi, Oudot 2017]

Contributions

Structure of Mapper depending on r, g, δ [C., Oudot 2016-17]

Heuristics and Statistics for Mapper [C., Michel, Oudot 2017]

Local Equivalence of Mapper and PDs [C., Oudot 2017]

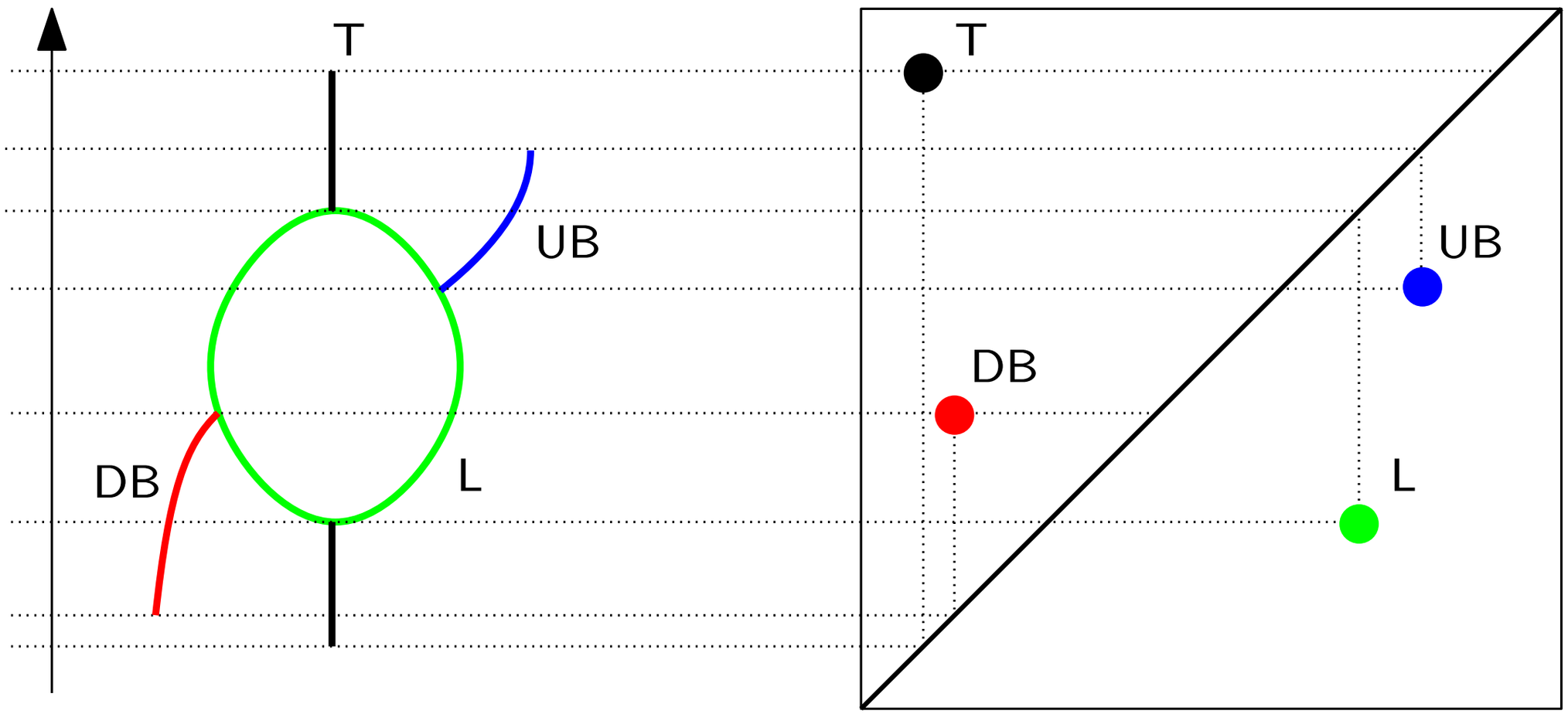
Machine Learning for Mapper (through PDs):

- Finite dimensional kernel [C., Ovsjanikov, Oudot 2015]
- Gaussian kernel [C., Cuturi, Oudot 2017]

Extended Persistence Diagram

Def: $\mathrm{Dg}(\mathrm{R}_f) =$ **bag-of-features** descriptor for $\mathrm{R}_f(X)$:

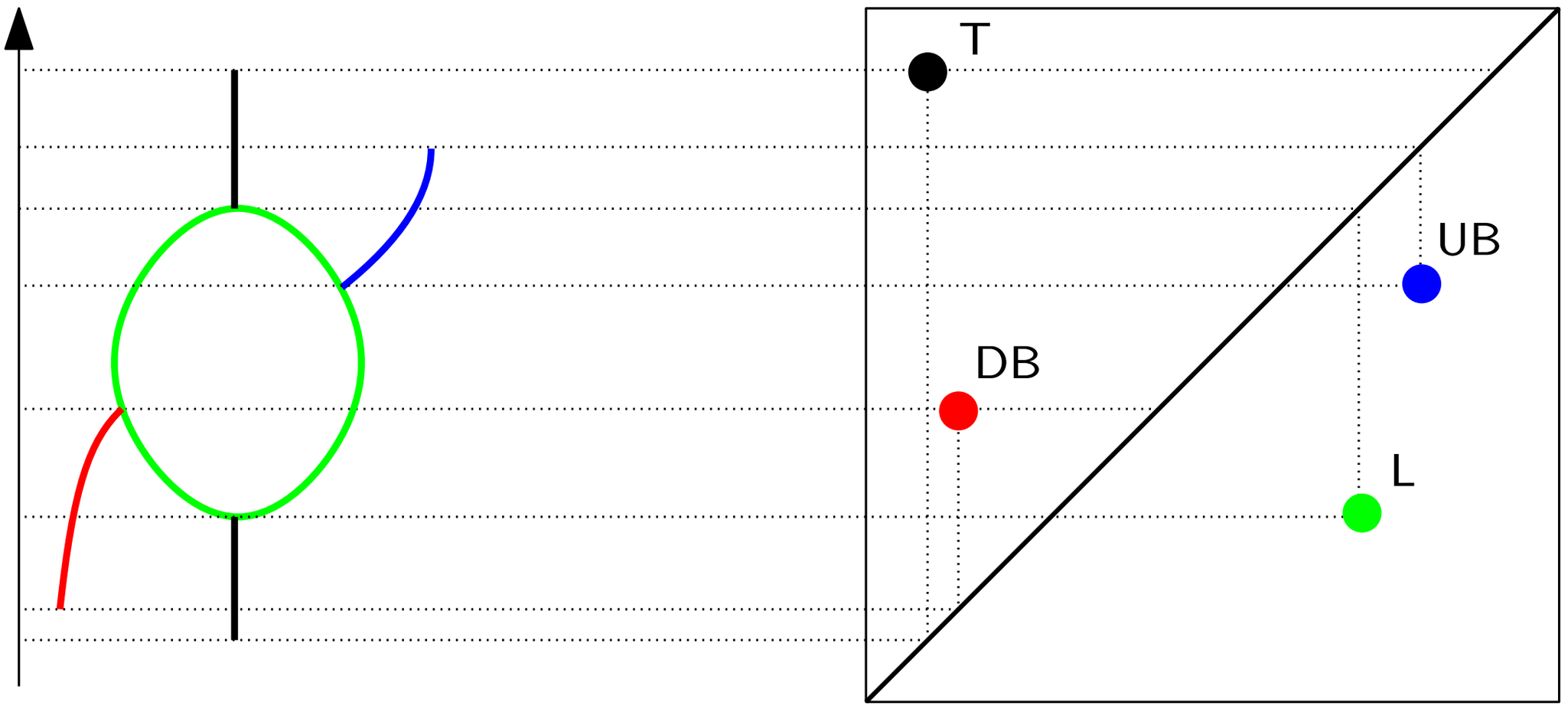
$\mathrm{DB}(\mathrm{R}_f) \longleftrightarrow$ downward branches	$\mathrm{T}(\mathrm{R}_f) \longleftrightarrow$ trunks (cc)
$\mathrm{UB}(\mathrm{R}_f) \longleftrightarrow$ upward branches	$\mathrm{L}(\mathrm{R}_f) \longleftrightarrow$ loops



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

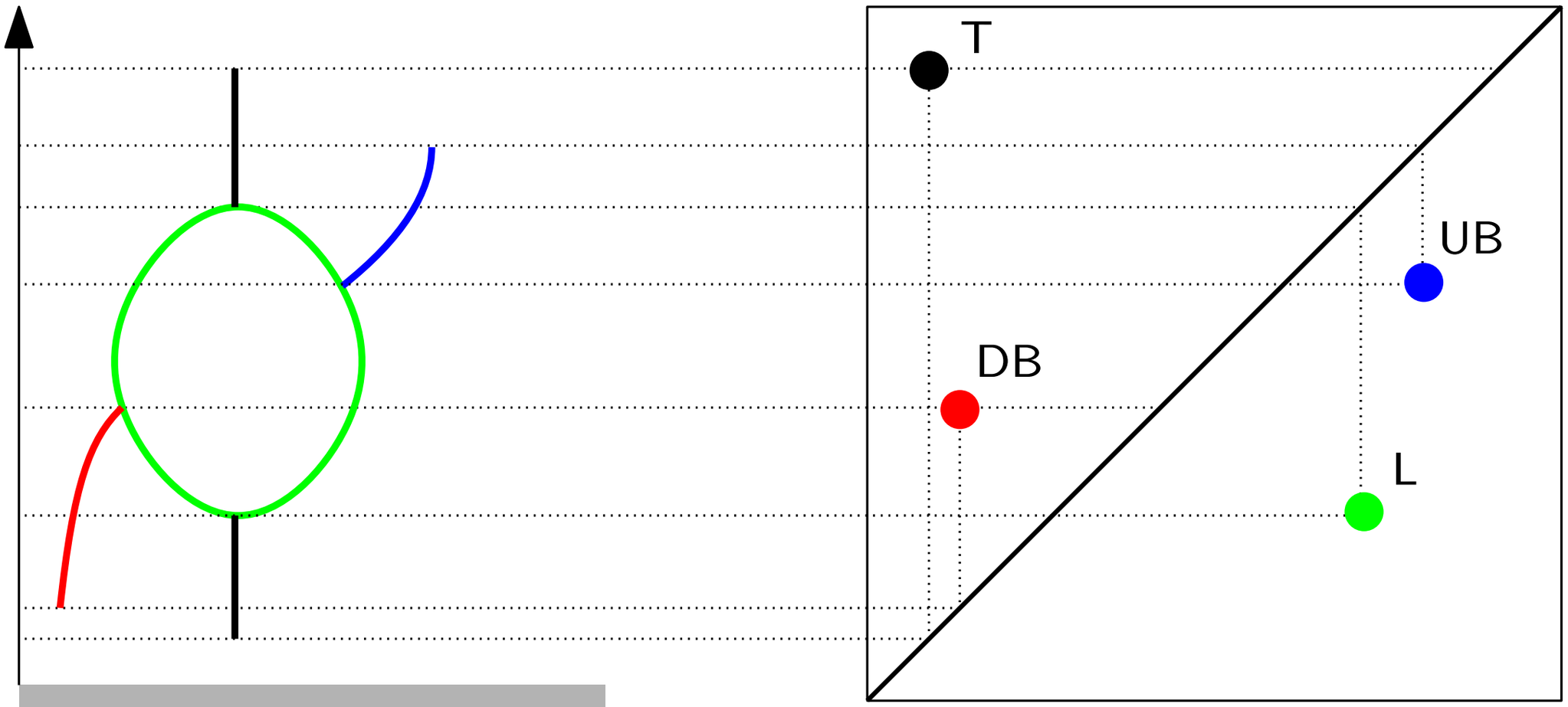
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

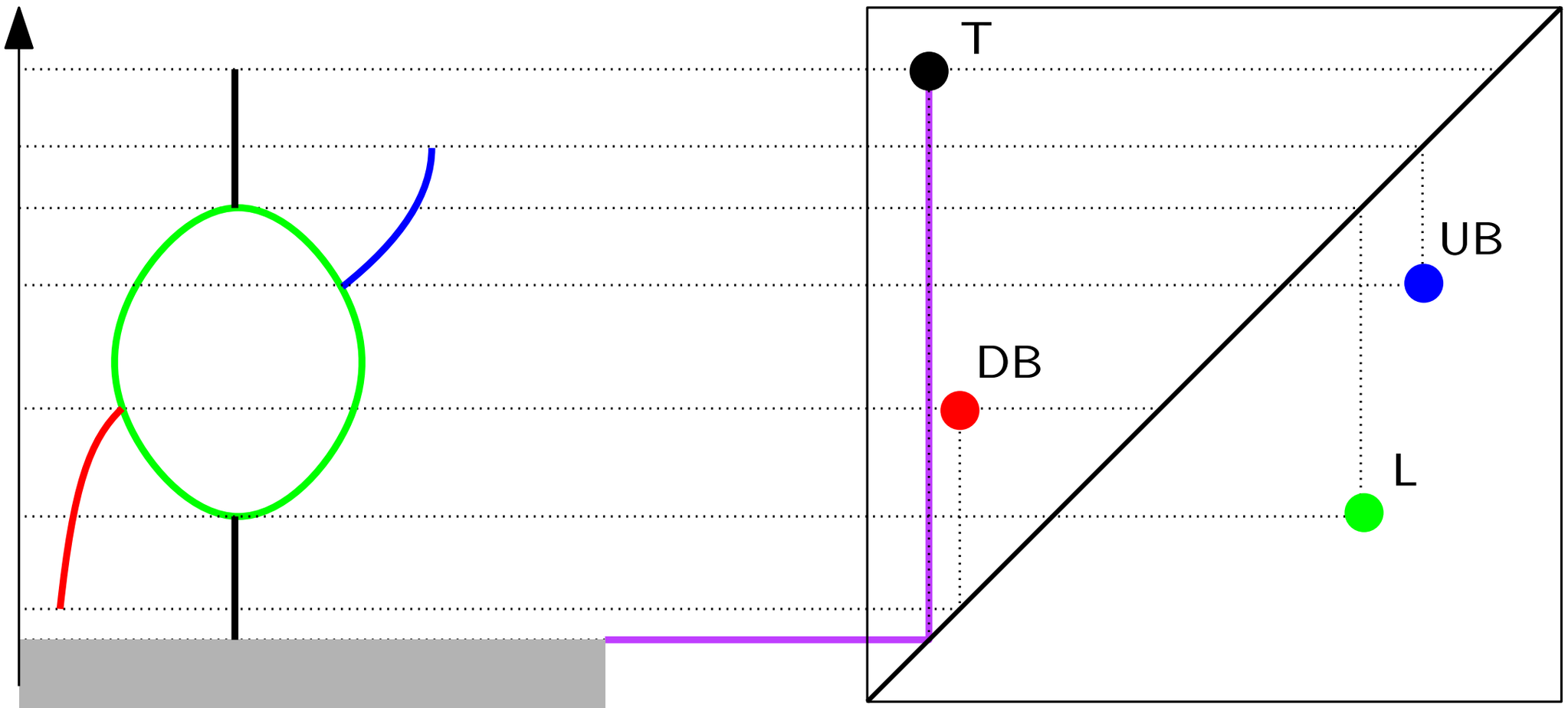
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

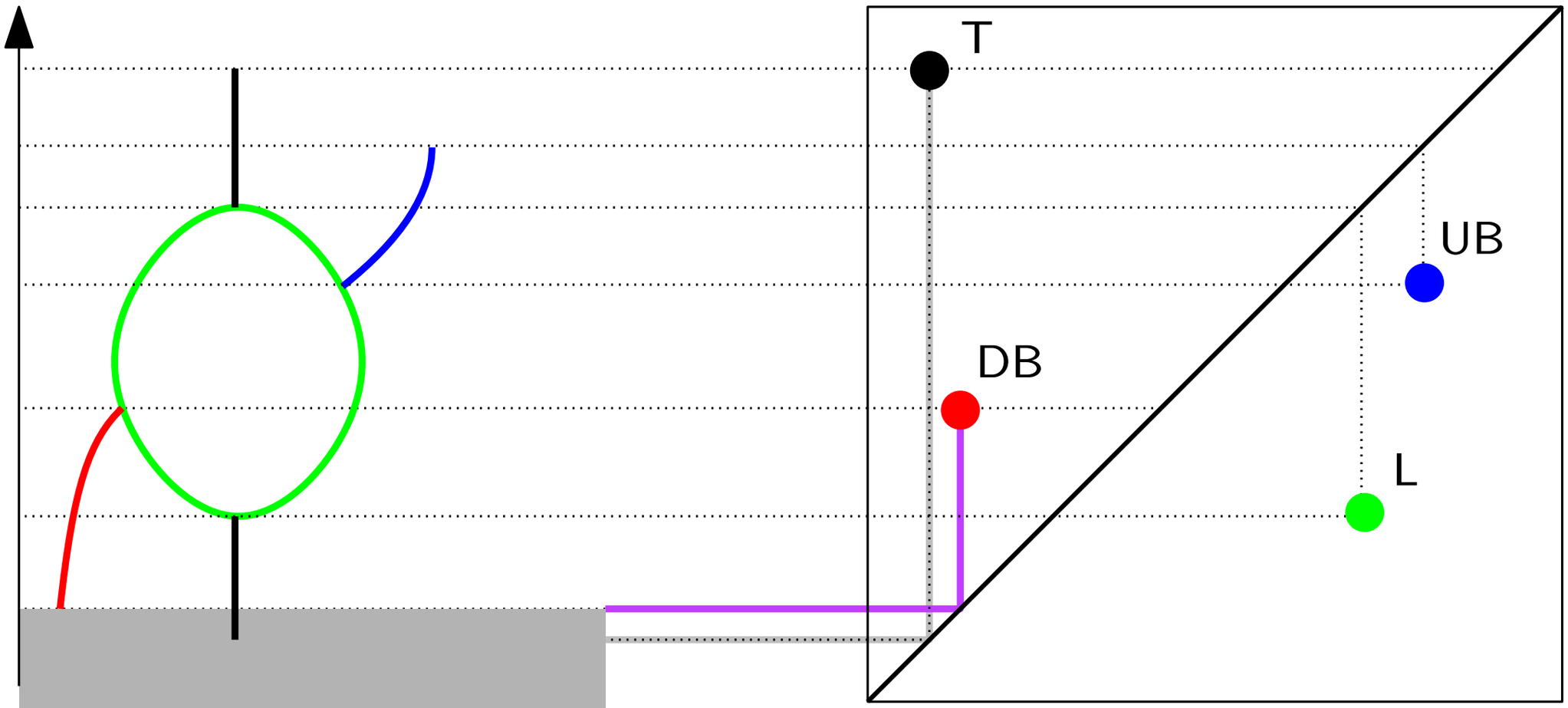
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

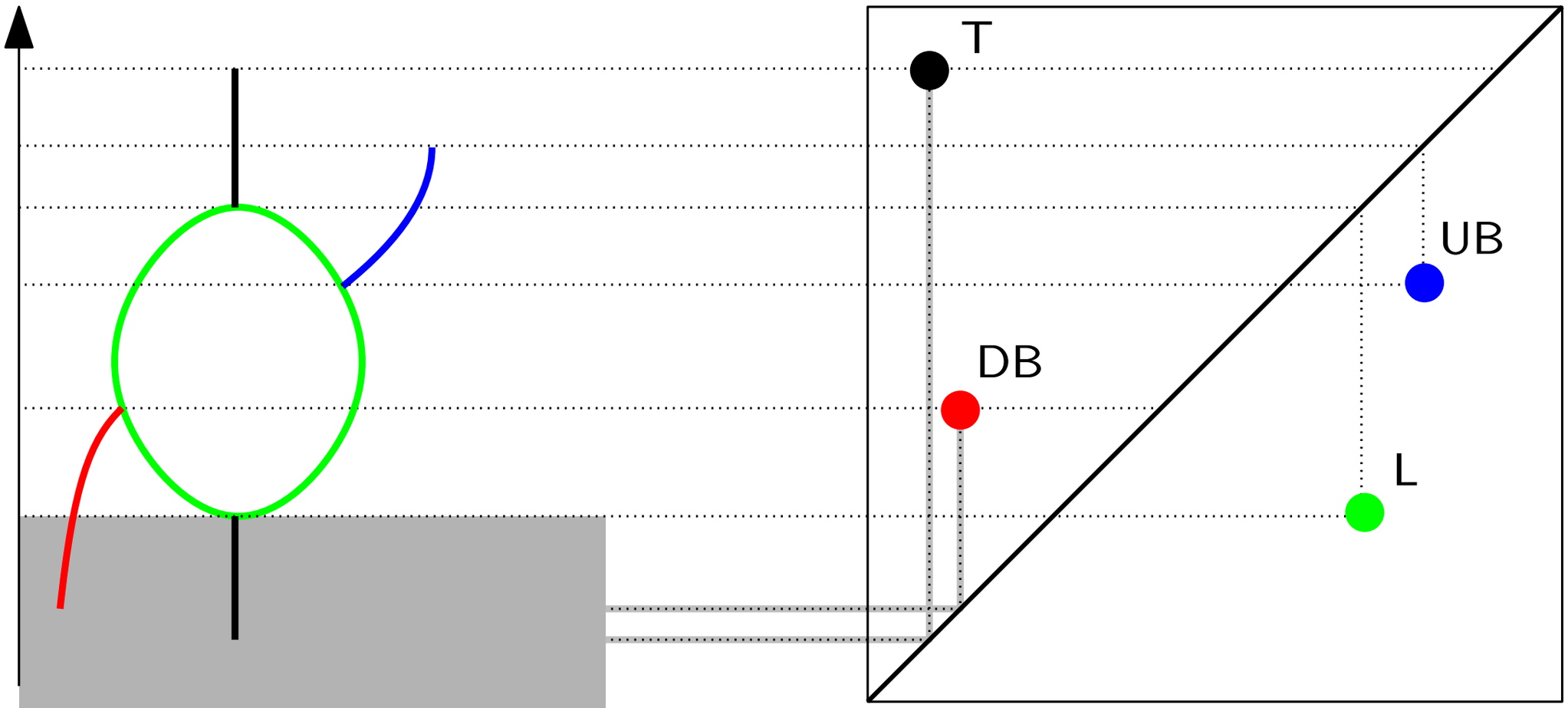
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

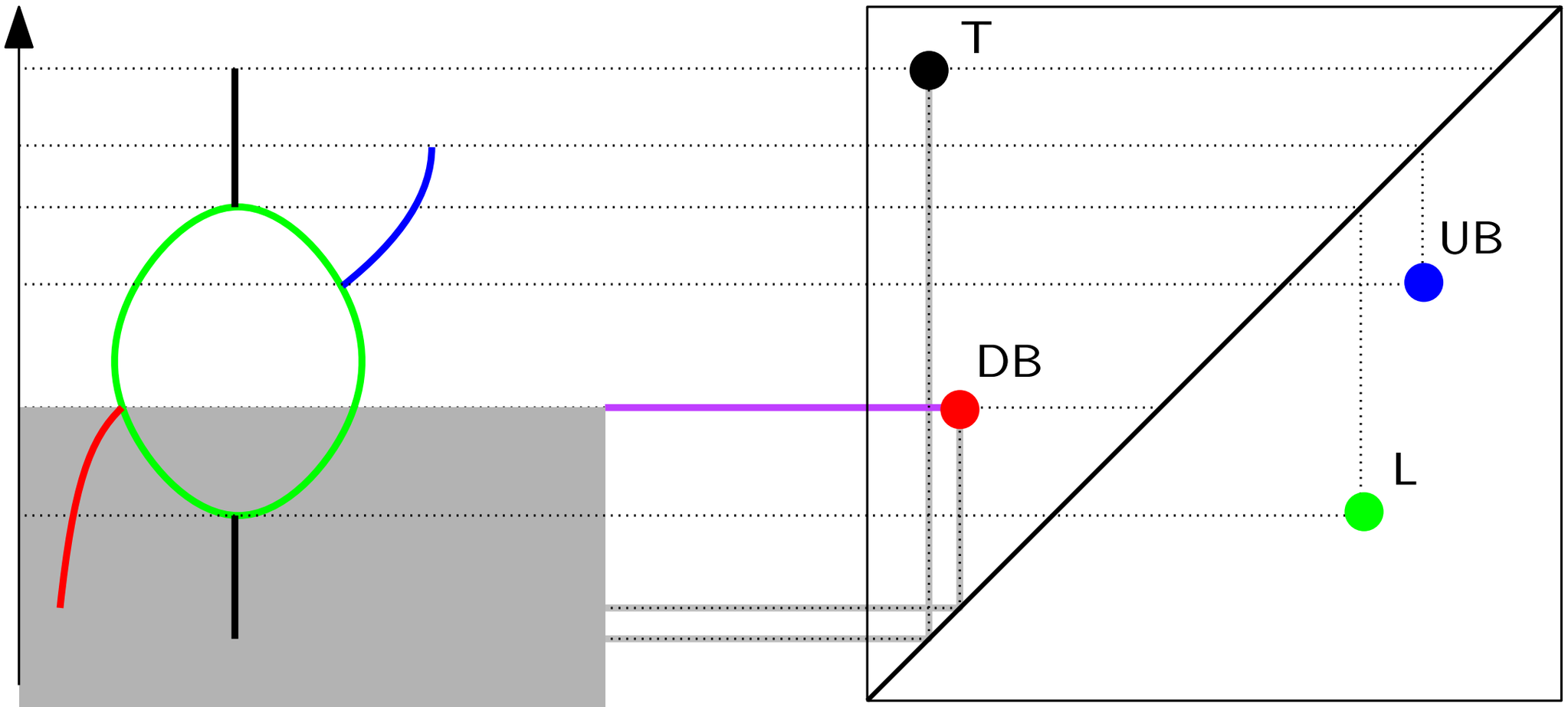
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

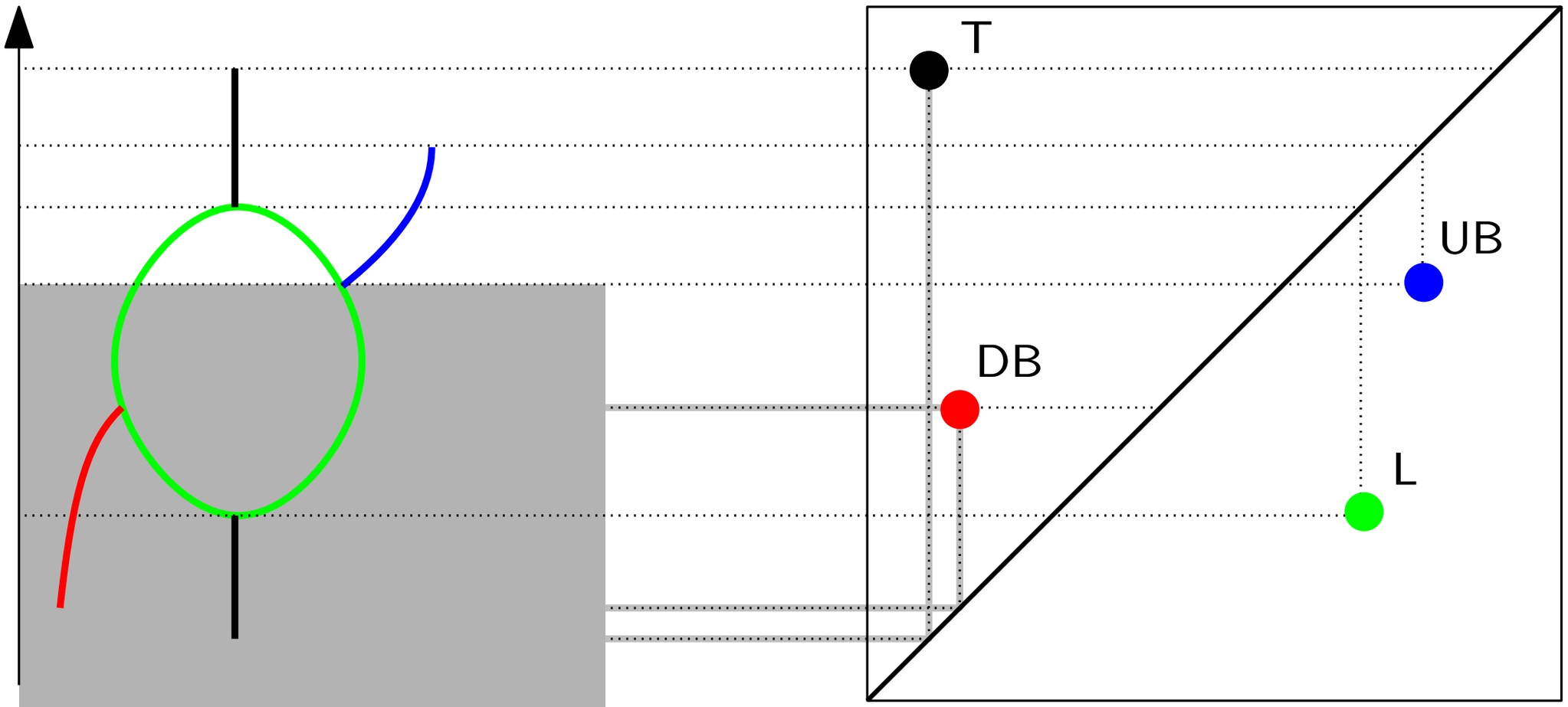
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

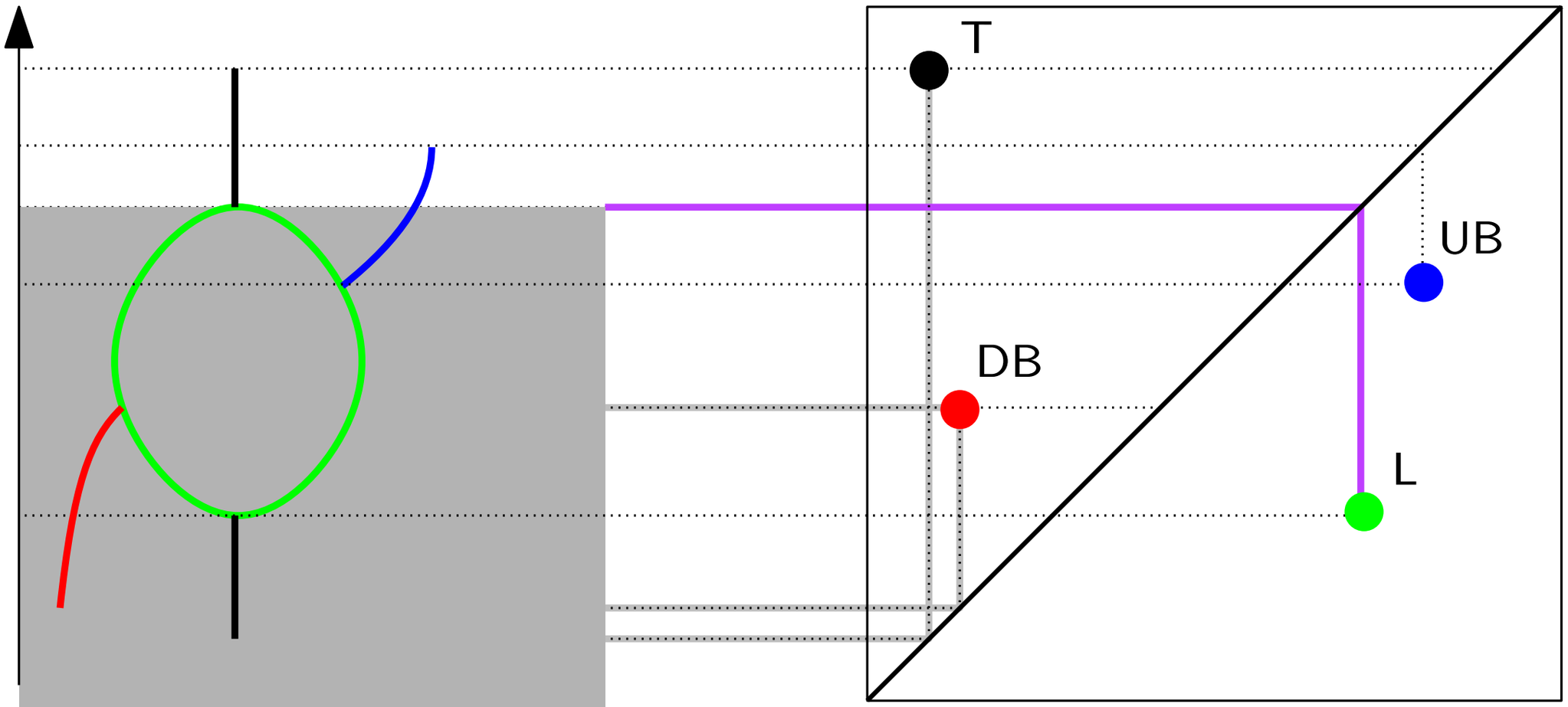
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

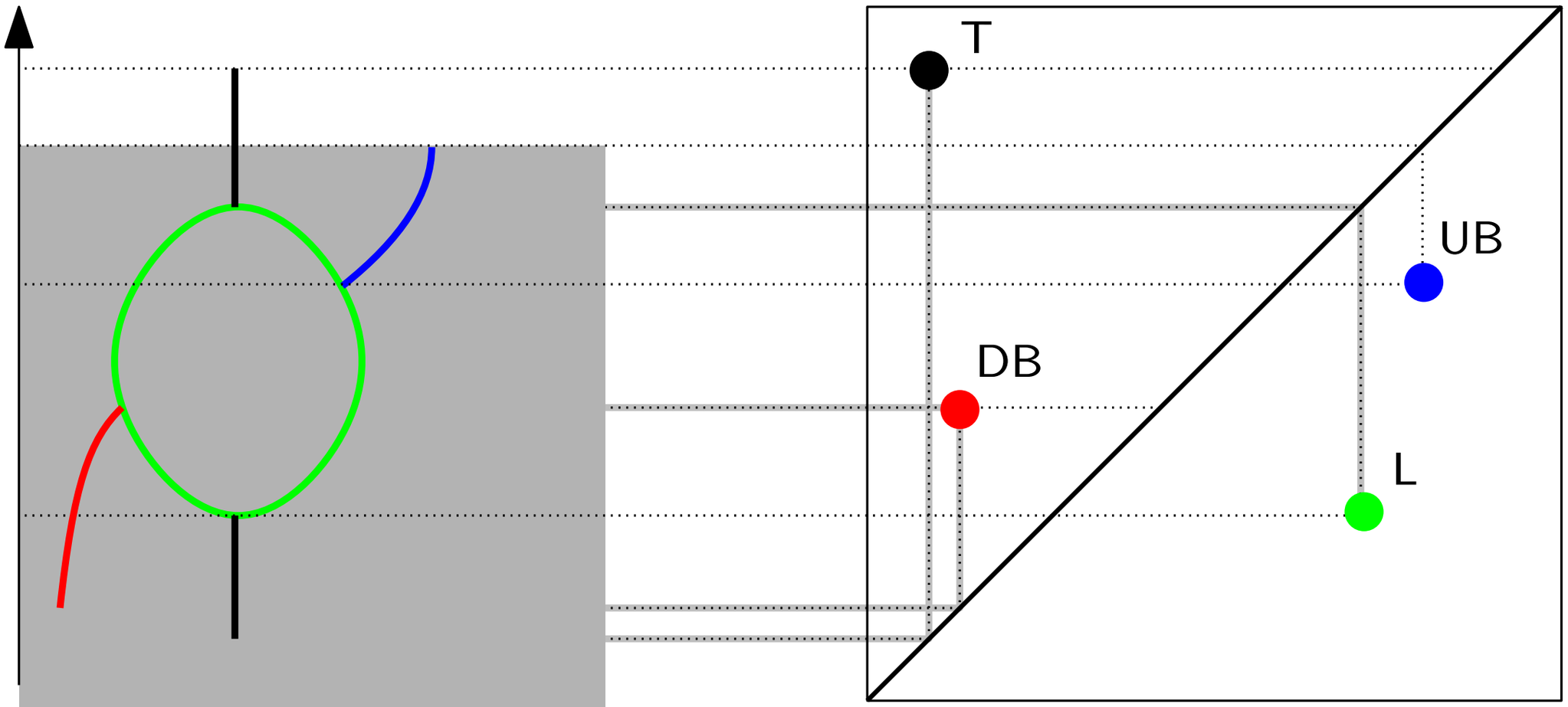
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

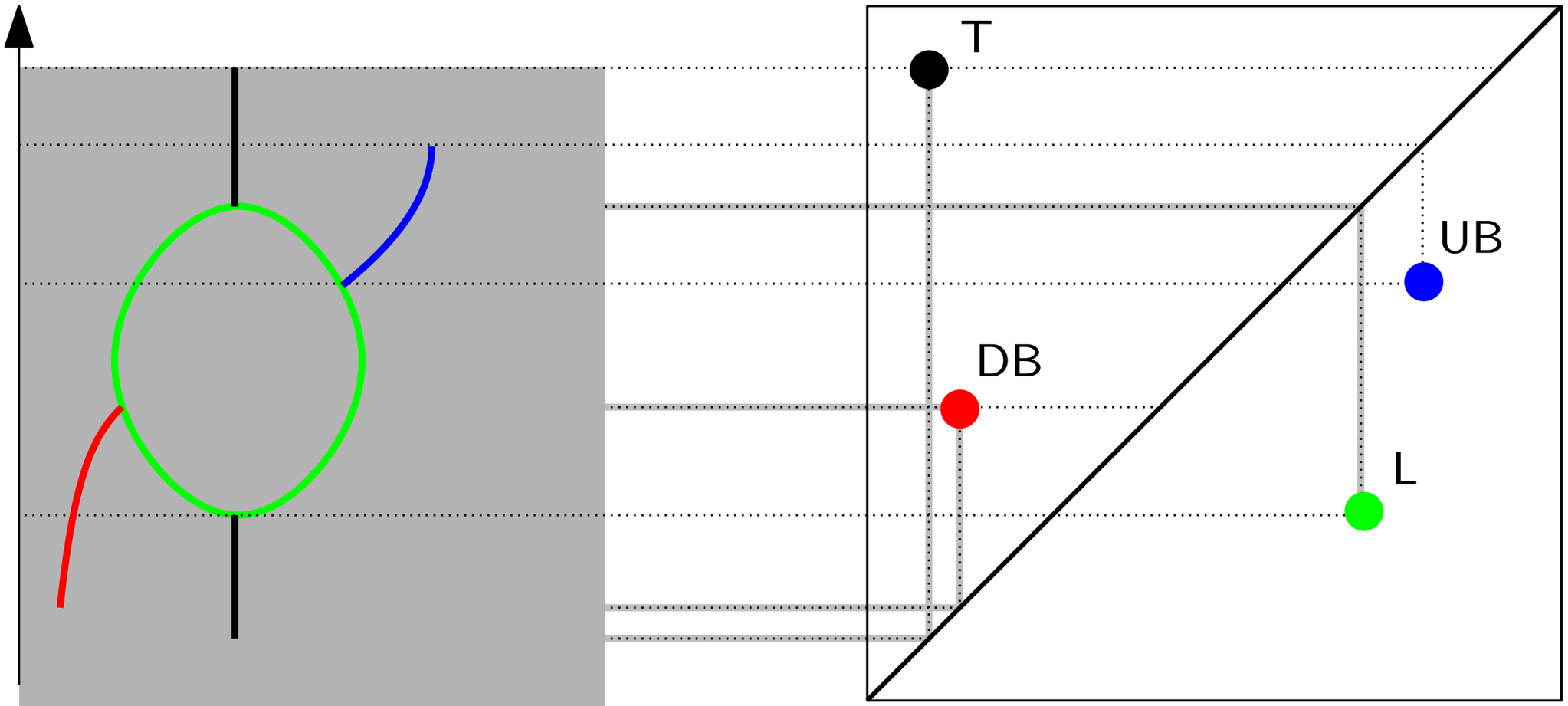
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

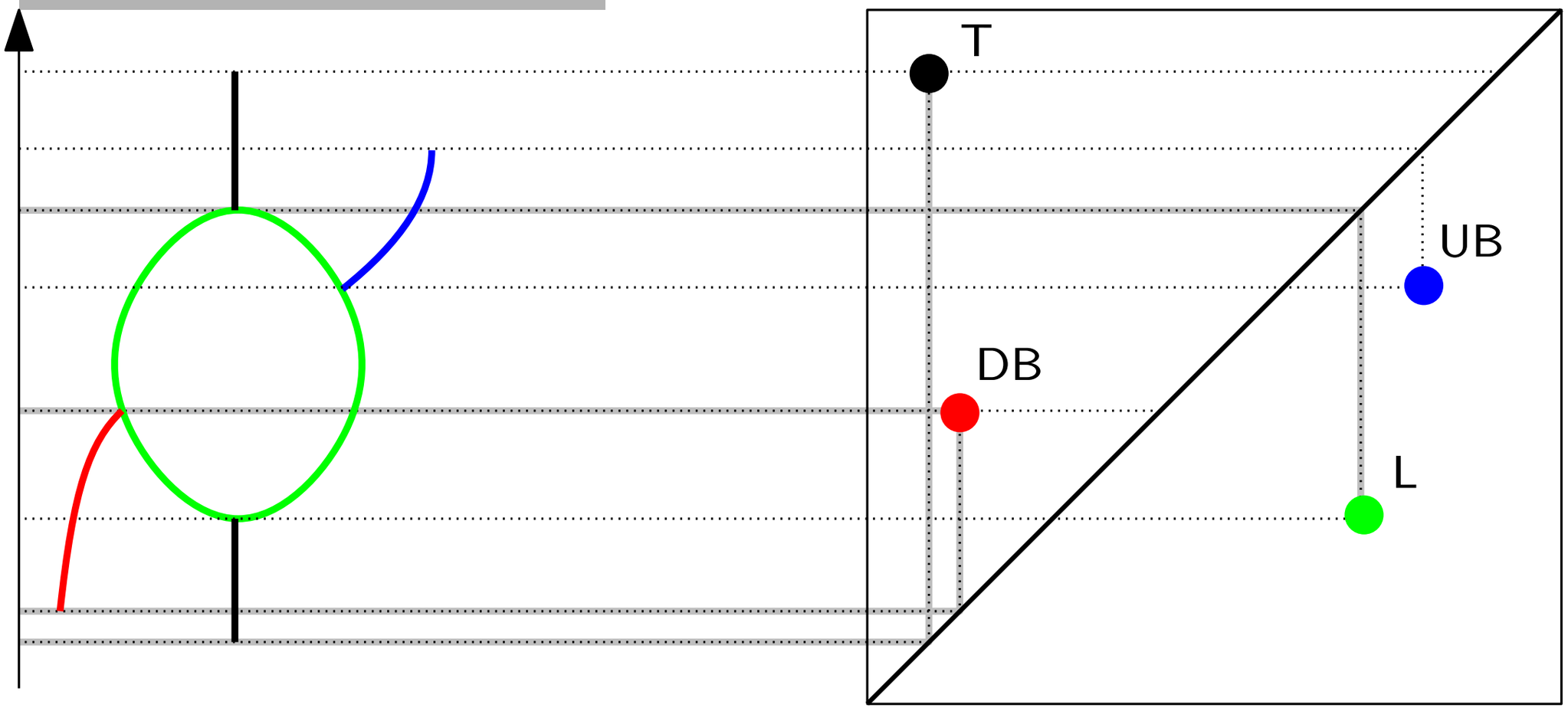
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

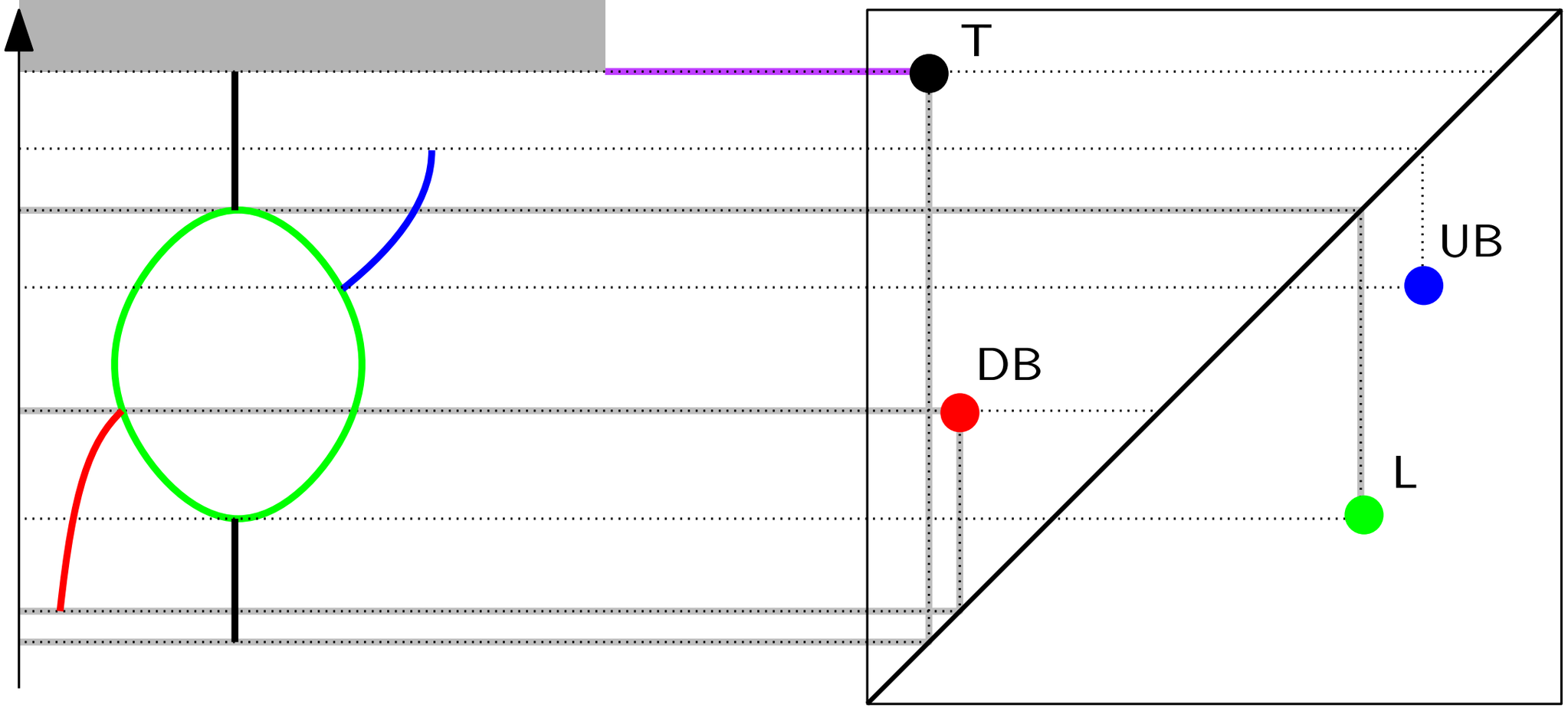
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

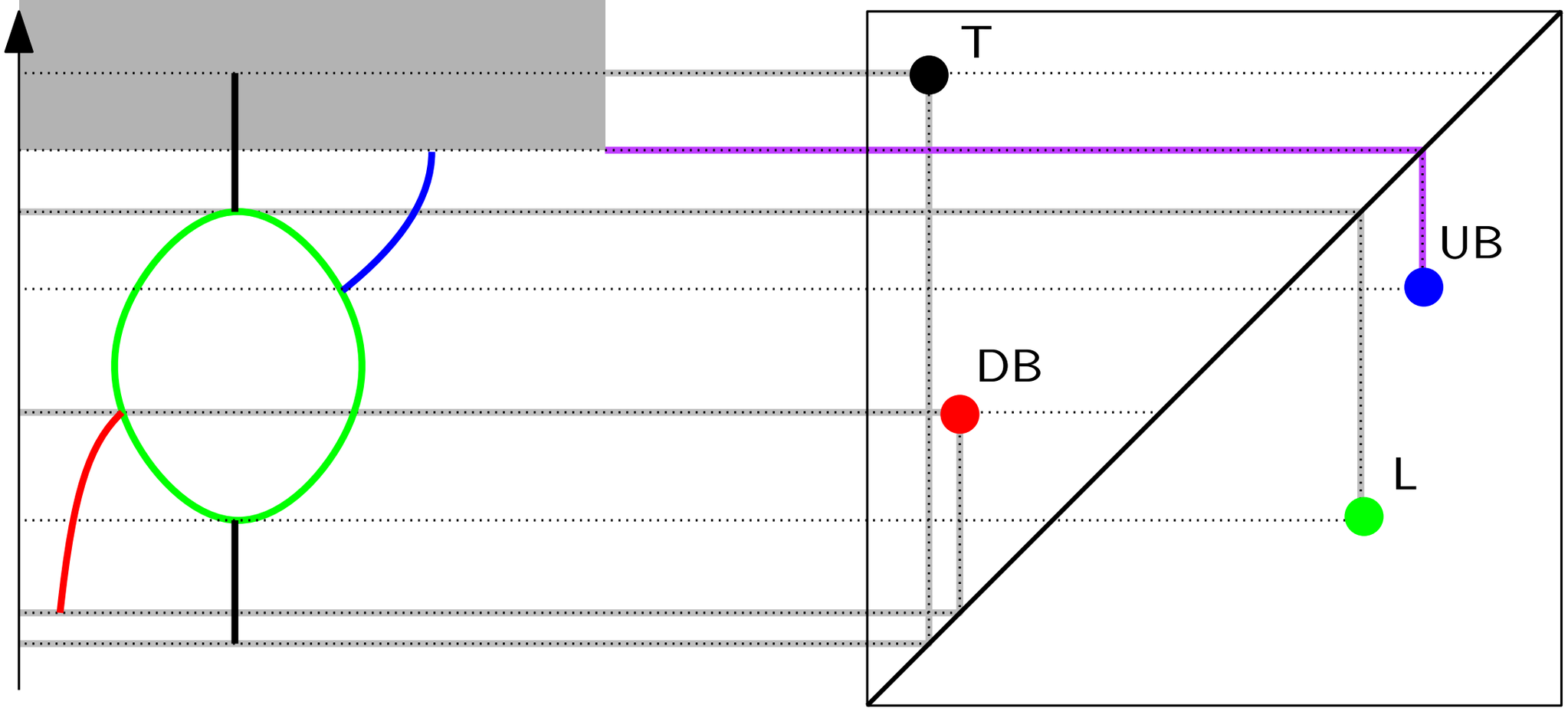
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

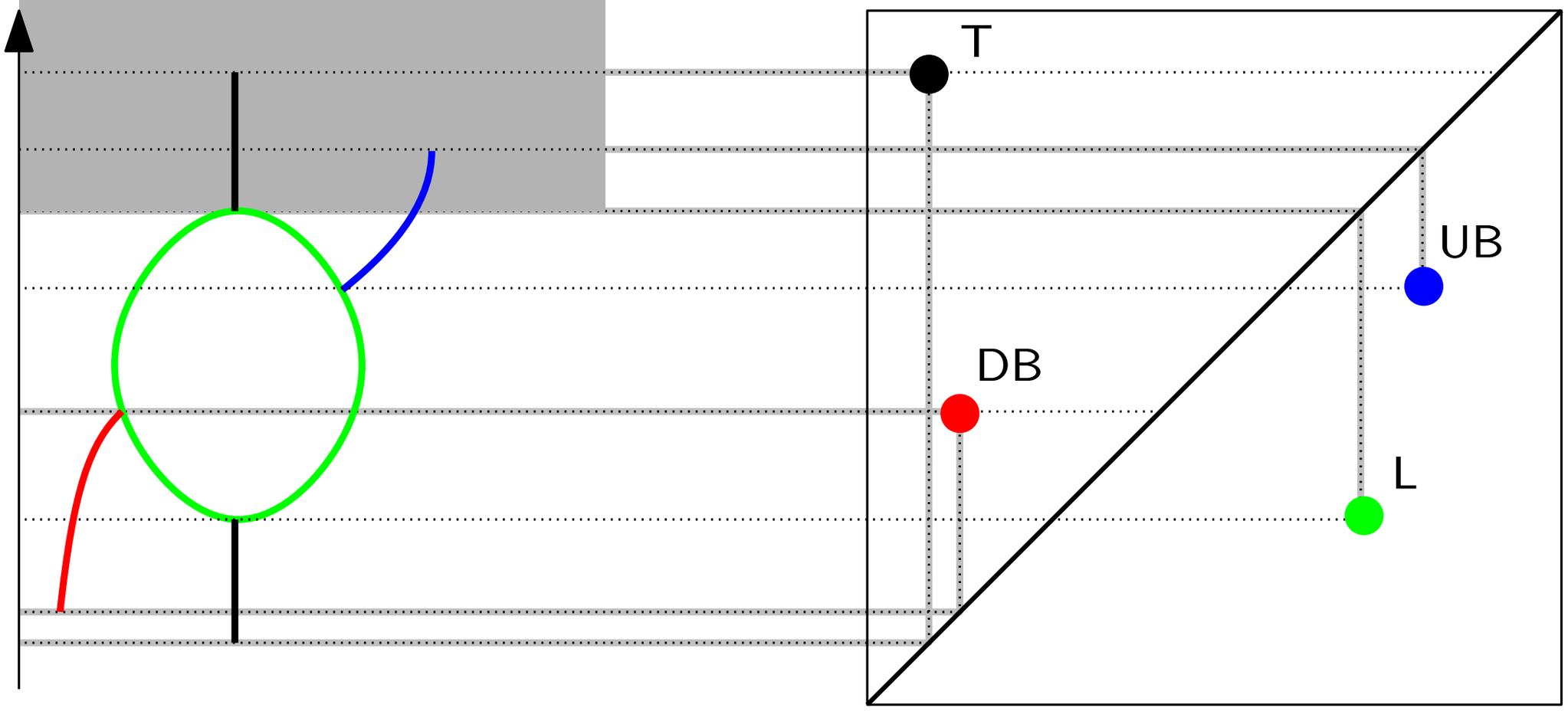
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

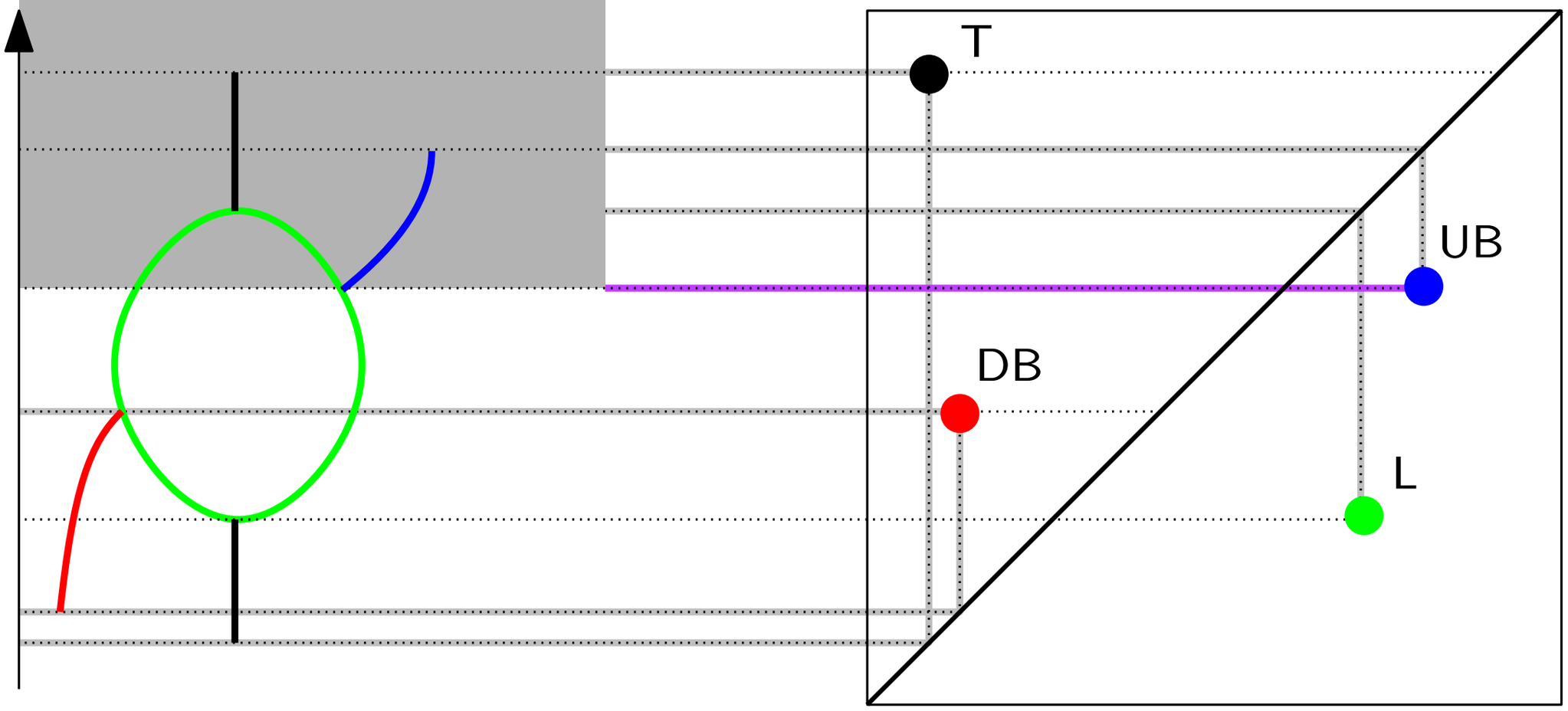
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

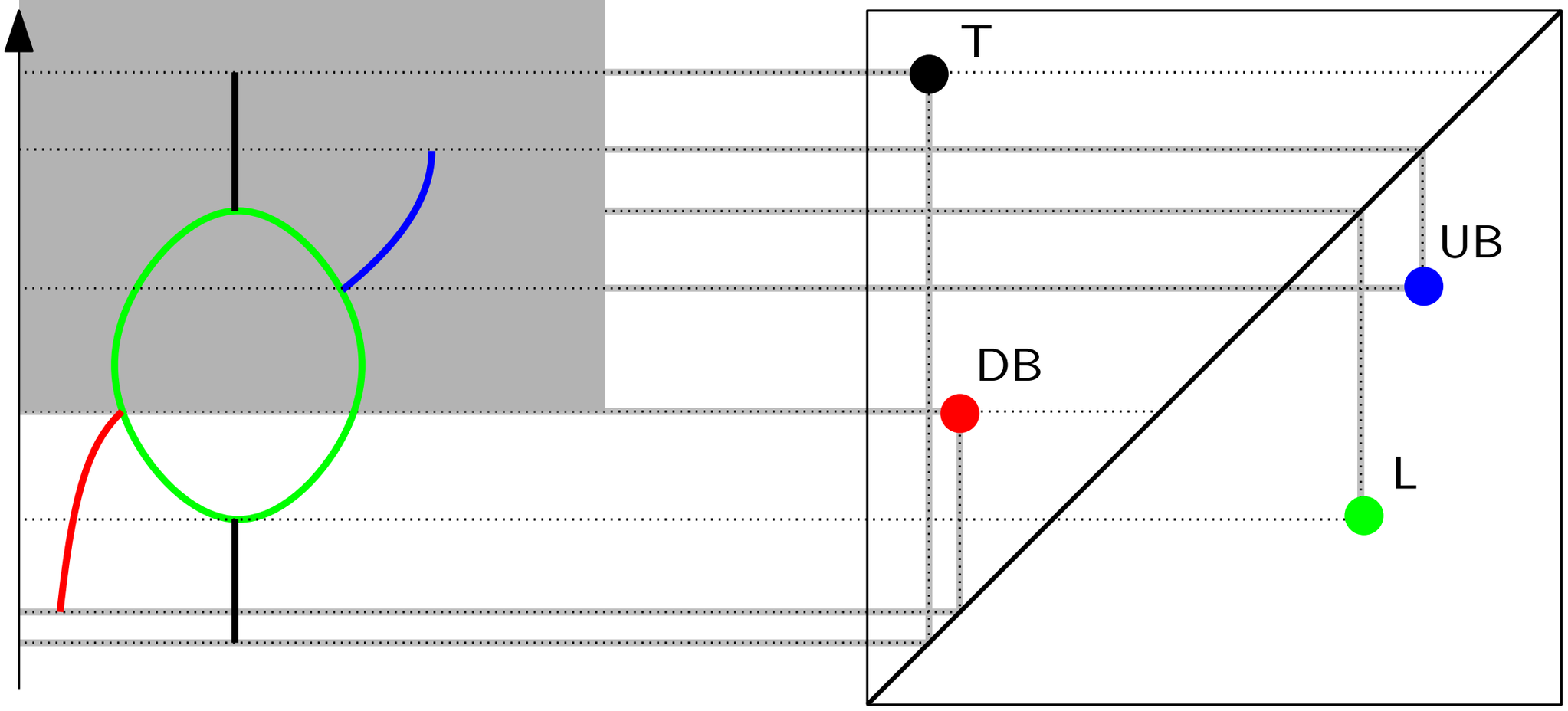
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

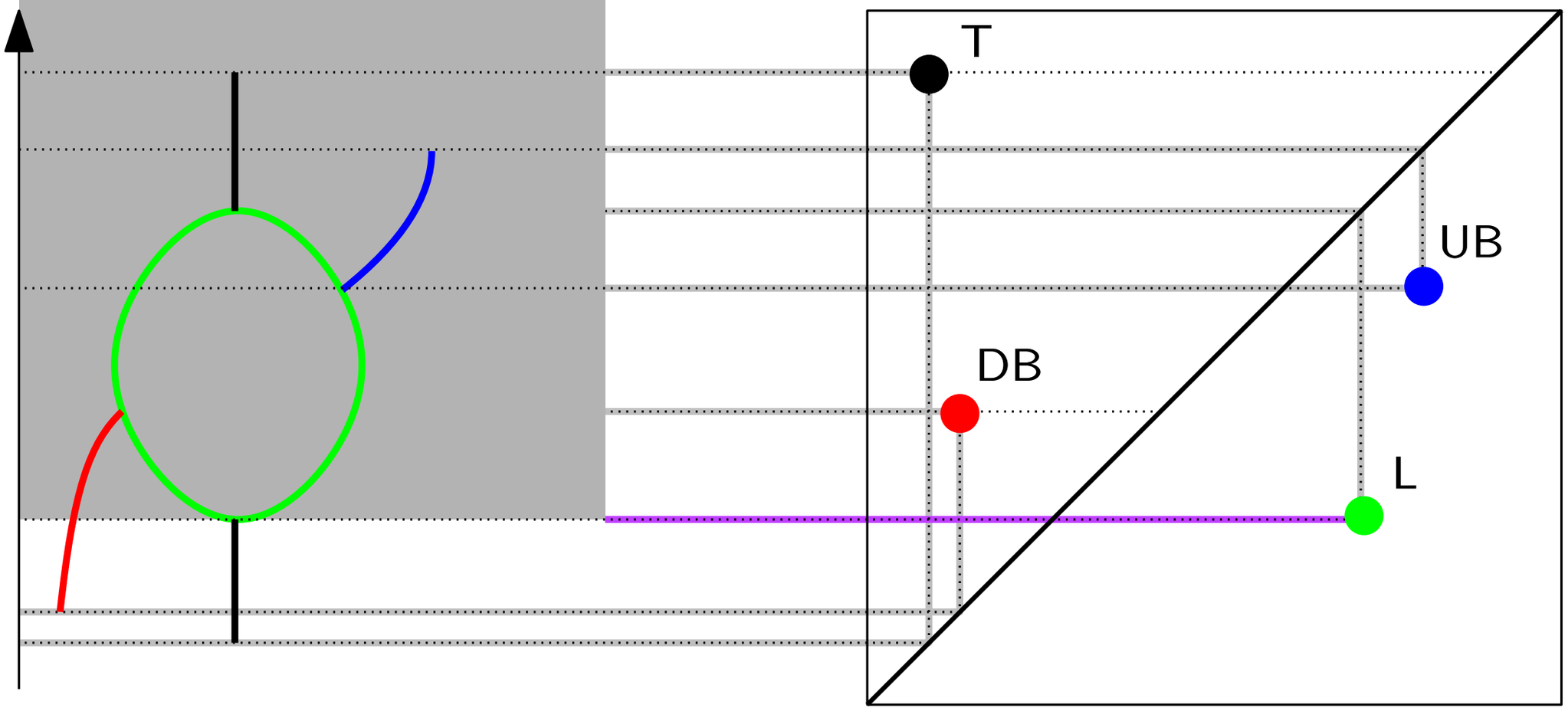
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

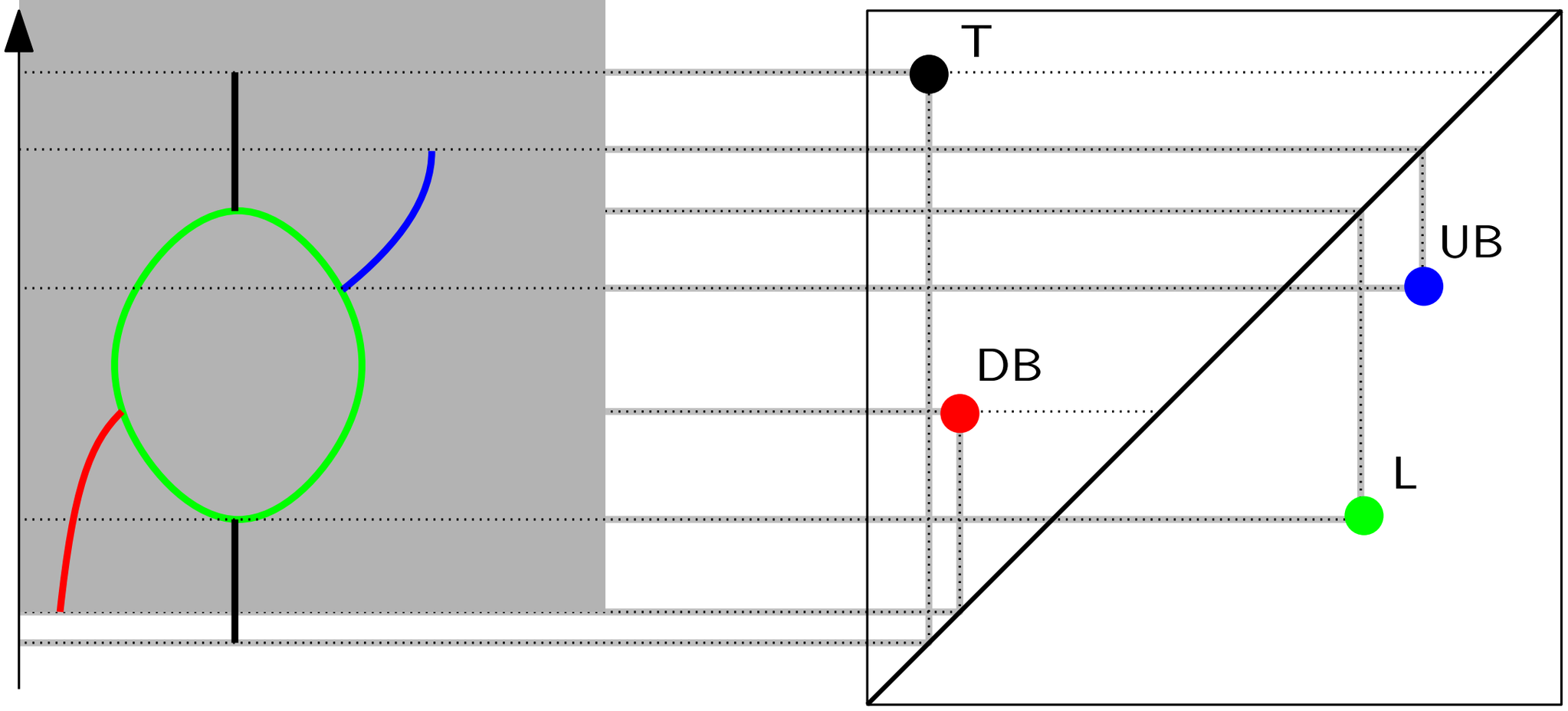
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

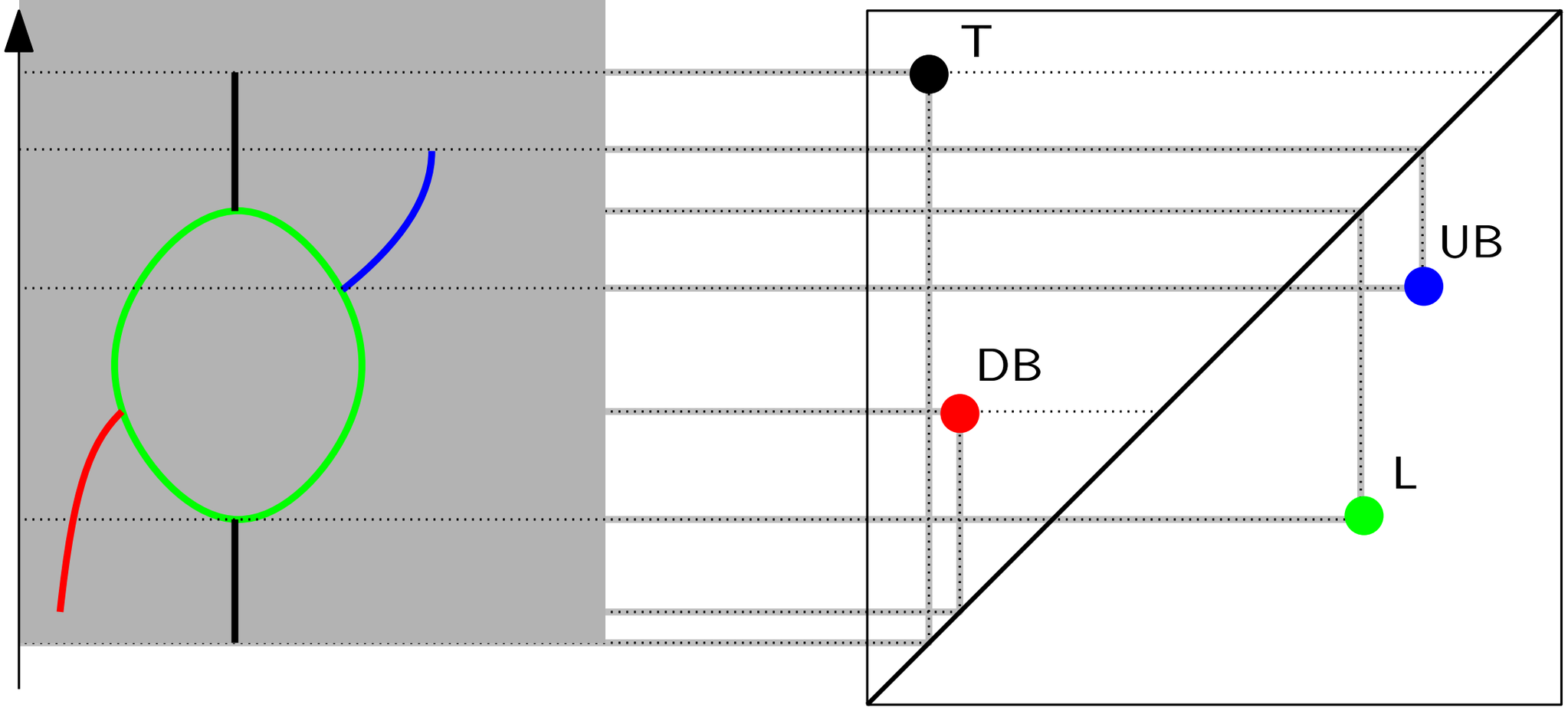
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

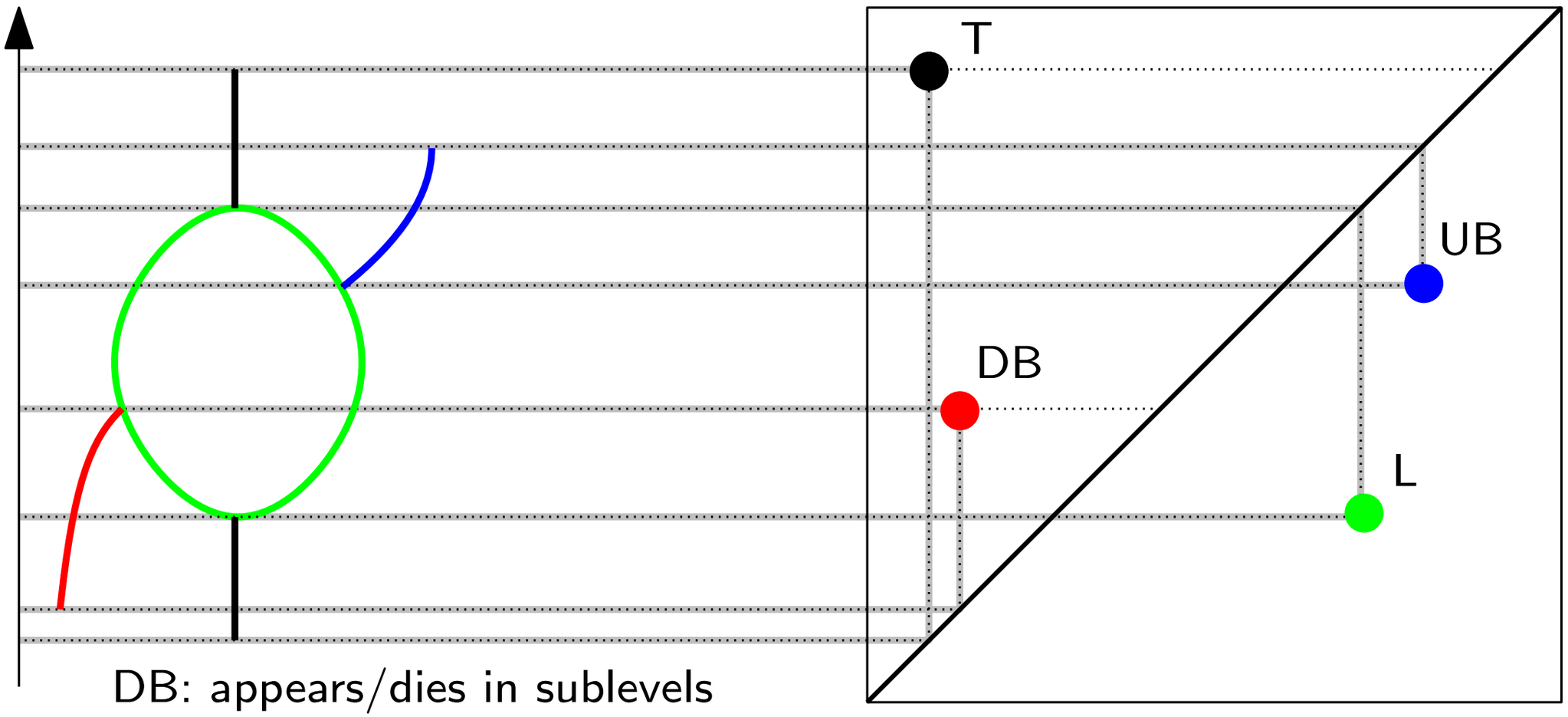
- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family



Extended Persistence Diagram

Construction uses **extended persistence**: [Cohen-Steiner, Edelsbrunner, Harer 2008]

- family of *excursion sets* (sublevel then superlevel sets) of Reeb graph
- use *homological algebra* to encode the evolution of the topology of the family

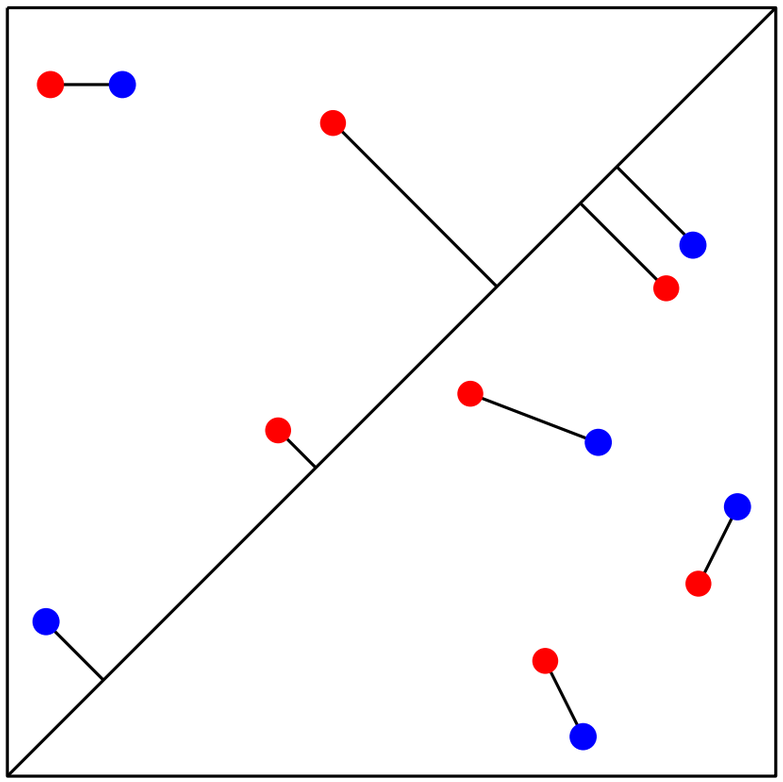


DB: appears/dies in sublevels

UB: appears/dies in superlevels

T/L: appears in sublevels, dies in superlevels

Metric for Extended Persistence Diagrams



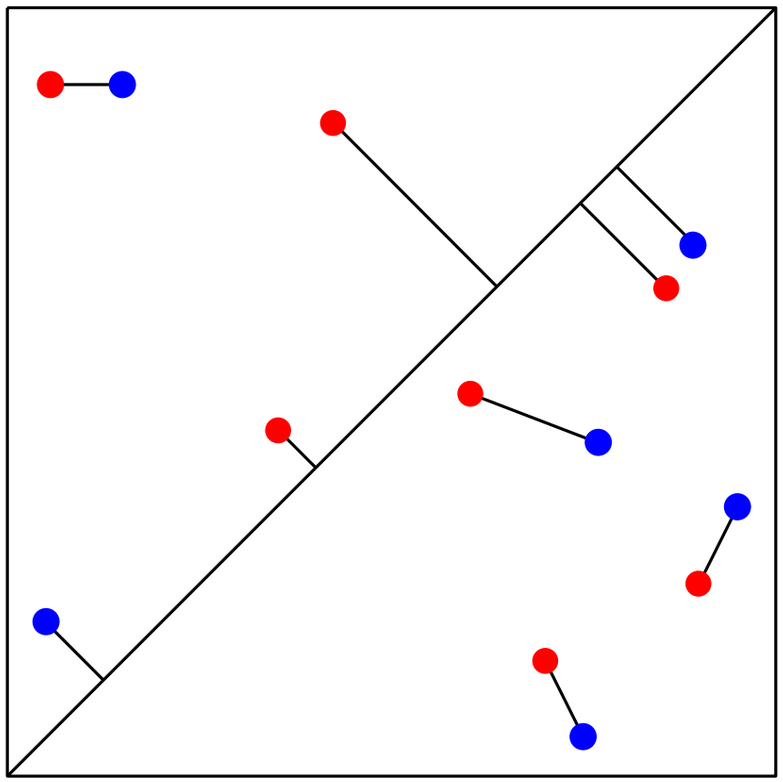
Metric for Extended Persistence Diagrams

Partial matching $M : \mathrm{Dg} \leftrightarrow \mathrm{Dg}'$

Matched pair $(x, y) \in M$: $c(x, y) = \|x - y\|_\infty$

Unmatched point $z \in X \sqcup Y$: $c(z) = \|z - \bar{z}\|_\infty$

$c(M) = \max\{\ \max_{(x,\,y)} c(x, y),\ \max_z c(z)\ \}$



Metric for Extended Persistence Diagrams

Partial matching $M : \mathrm{Dg} \leftrightarrow \mathrm{Dg}'$

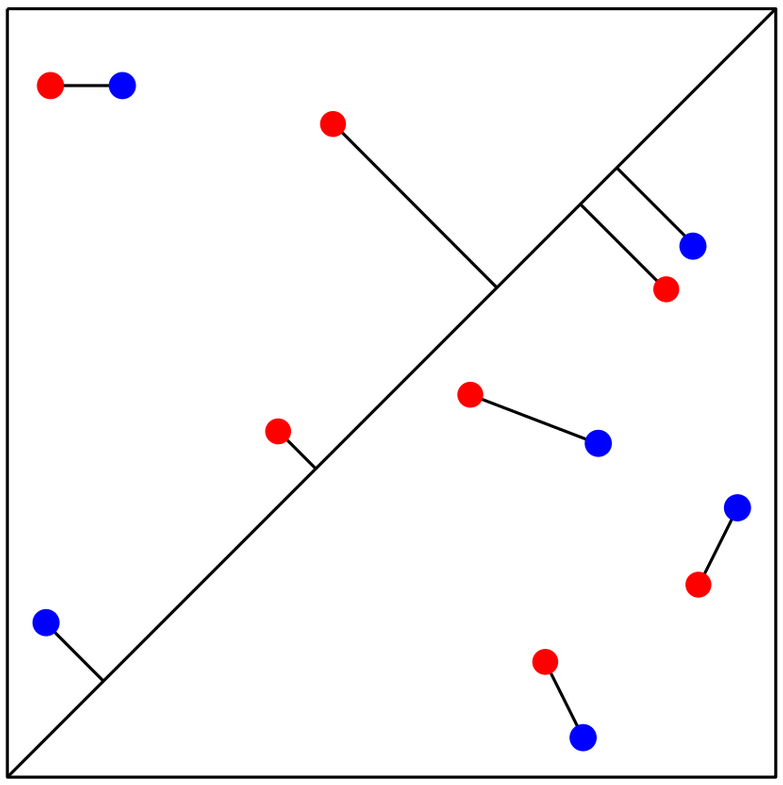
Matched pair $(x, y) \in M$: $c(x, y) = \|x - y\|_\infty$

Unmatched point $z \in X \sqcup Y$: $c(z) = \|z - \bar{z}\|_\infty$

$c(M) = \max\{ \max_{(x,\, y)} c(x, y),\ \max_z c(z) \}$

Def: bottleneck distance:

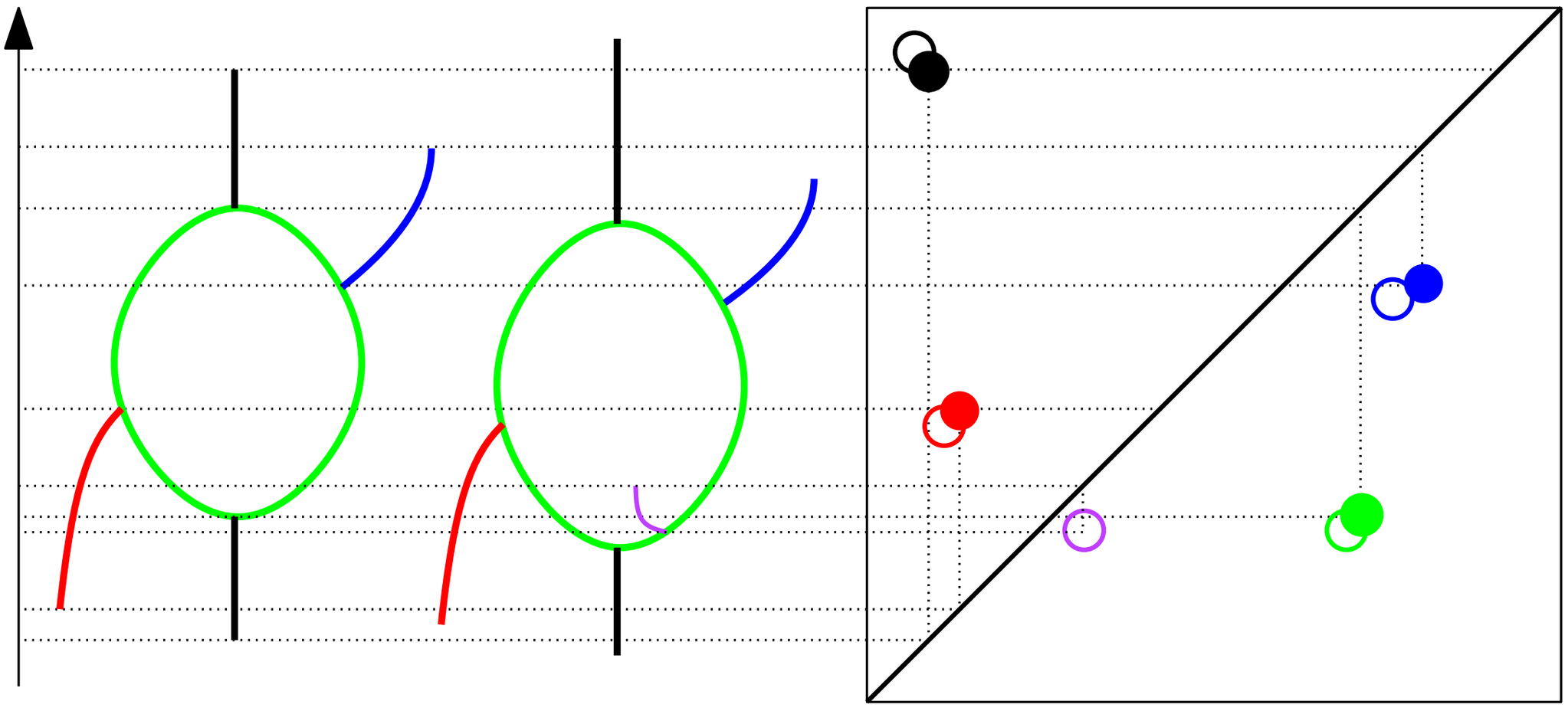
$$\mathrm{d}_B(\mathrm{Dg}, \mathrm{Dg}') = \inf_{M : \mathrm{Dg} \leftrightarrow \mathrm{Dg}'} c(M)$$



Metric Properties

Thm (stability): [Bauer, Ge, Wang 2013]

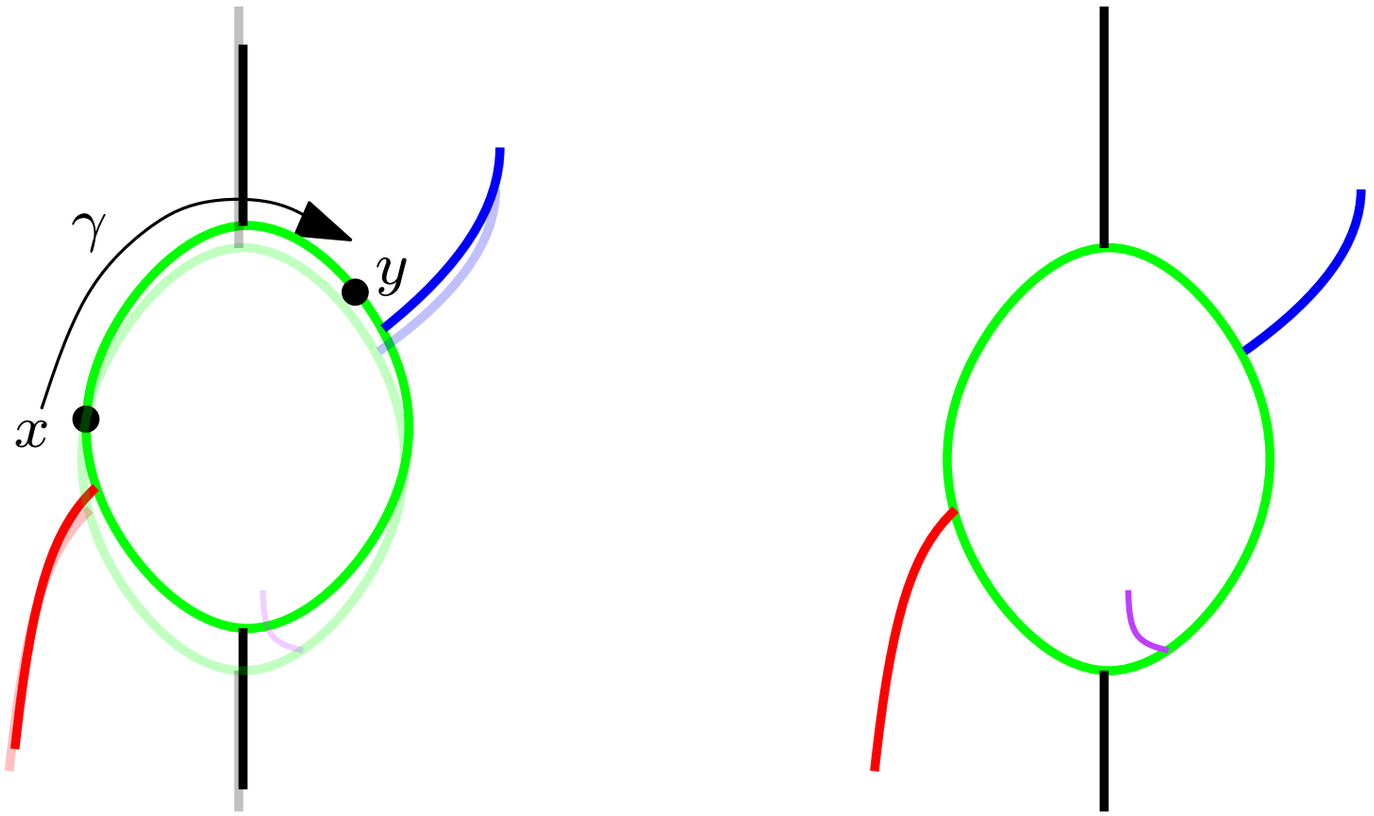
$$\mathrm{d}_B(\mathrm{Dg}\,(\mathrm{R}_f), \mathrm{Dg}\,(\mathrm{R}_g)) \leq 6\,\mathrm{d}_{\mathrm{GH}}(\mathrm{R}_f, \mathrm{R}_g)$$



Metric Properties

Thm (stability): [Bauer, Ge, Wang 2013]

$$\mathrm{d}_B(\mathrm{Dg}\,(\mathrm{R}_f), \mathrm{Dg}\,(\mathrm{R}_g)) \leq 6\,\mathrm{d}_{\mathrm{GH}}(\mathrm{R}_f, \mathrm{R}_g)$$

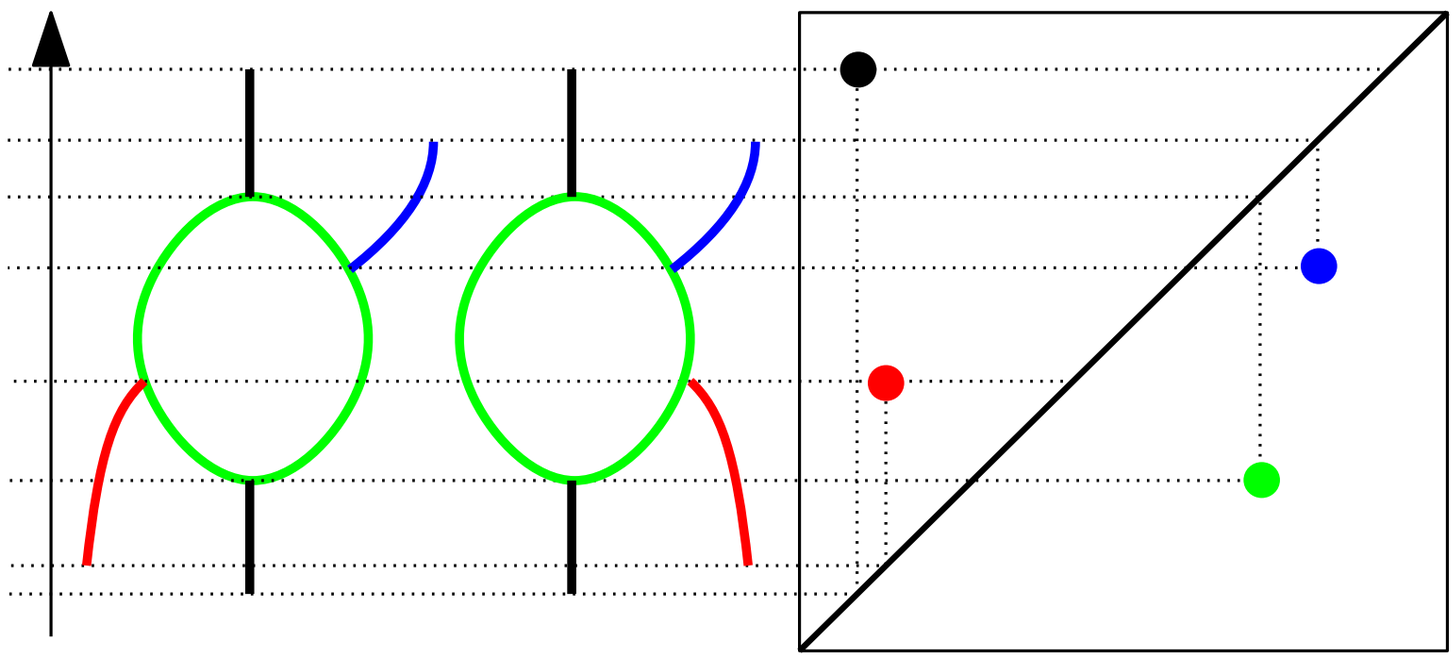


Metric Properties

Thm (stability): [Bauer, Ge, Wang 2013]

$$\mathrm{d}_B(\mathrm{Dg}\,(\mathrm{R}_f), \mathrm{Dg}\,(\mathrm{R}_g)) \leq 6\,\mathrm{d}_{\mathrm{GH}}(\mathrm{R}_f, \mathrm{R}_g)$$

Note: $\mathrm{d}_B(\mathrm{Dg}\,(\cdot), \mathrm{Dg}\,(\cdot))$ is only a pseudometric on Reeb graphs



Metric Properties

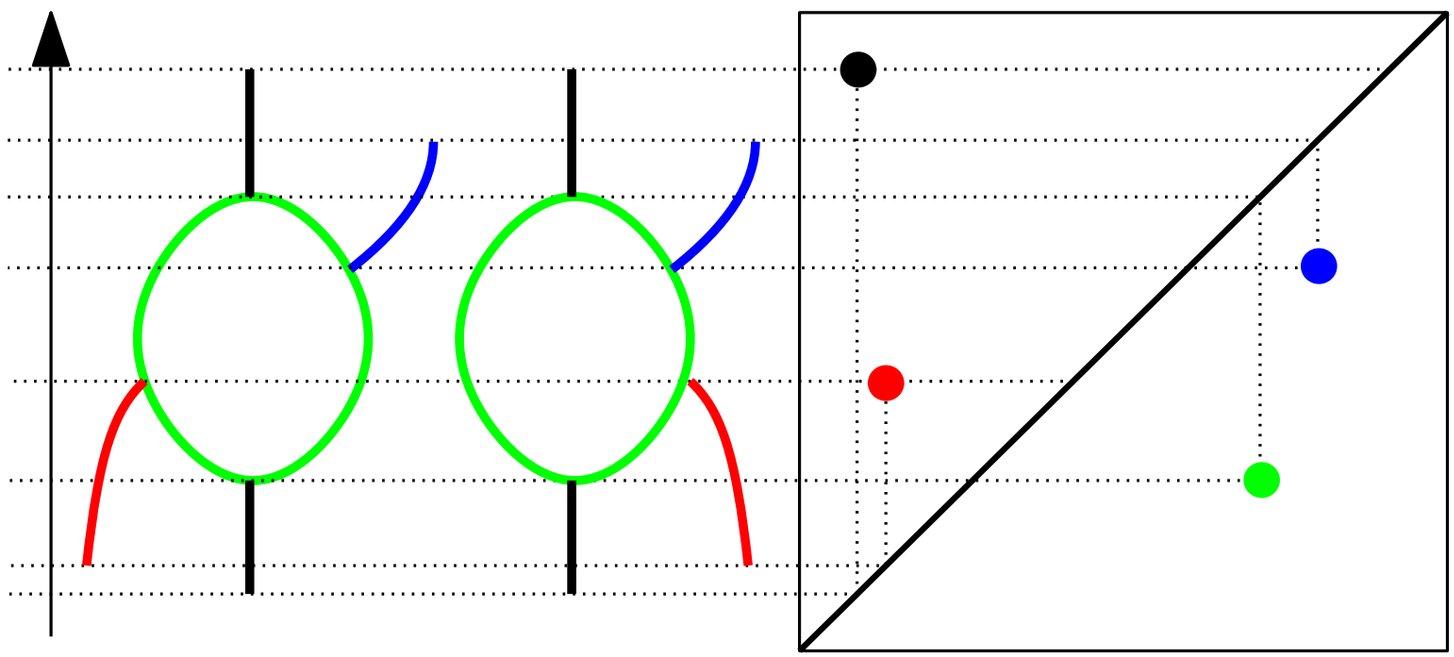
Thm (stability): [Bauer, Ge, Wang 2013]

$$\mathrm{d}_B(\mathrm{Dg}\,(\mathrm{R}_f), \mathrm{Dg}\,(\mathrm{R}_g)) \leq 6\,\mathrm{d}_{\mathrm{GH}}(\mathrm{R}_f, \mathrm{R}_g)$$

Note: $\mathrm{d}_B(\mathrm{Dg}\,(\cdot), \mathrm{Dg}\,(\cdot))$ is only a pseudometric on Reeb graphs

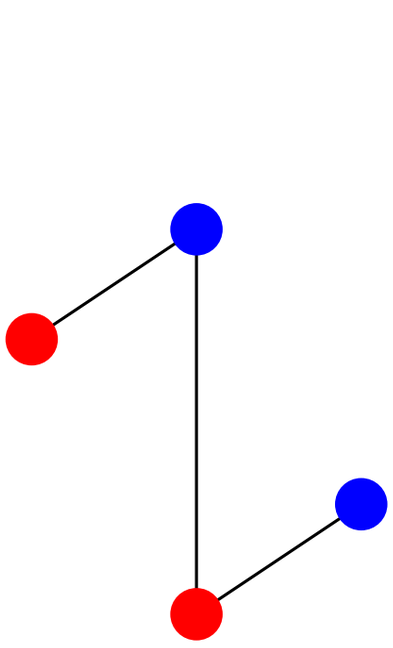
Thm: [C., Oudot 2016]

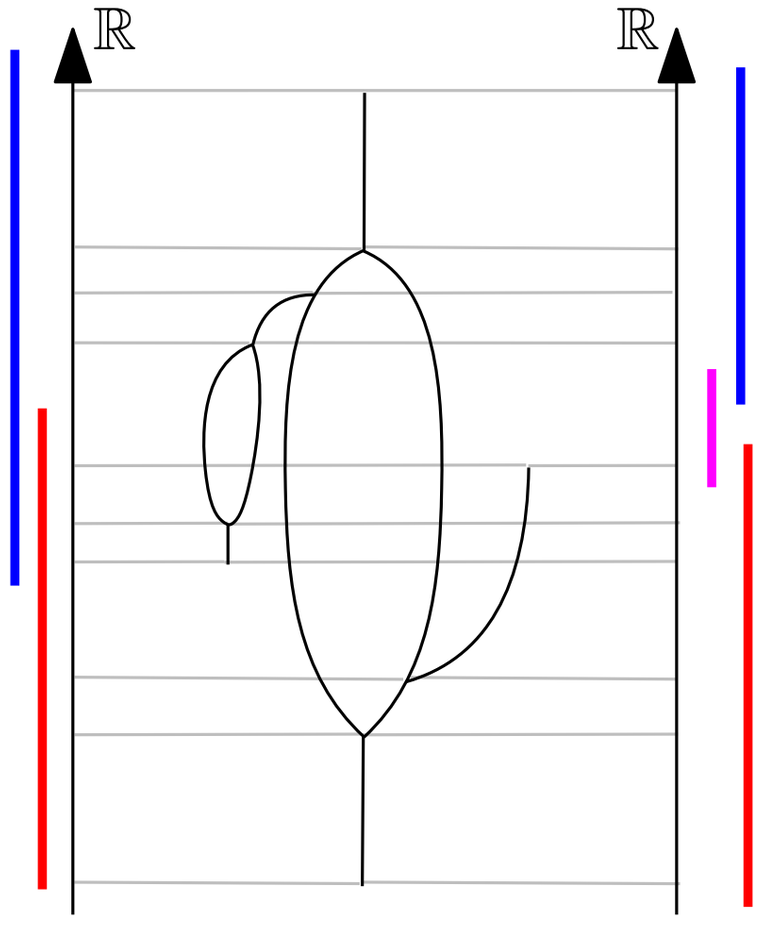
$\mathrm{d}_B(\mathrm{Dg}\,(\cdot), \mathrm{Dg}\,(\cdot))$ is *locally* a metric equivalent to d_{GH}

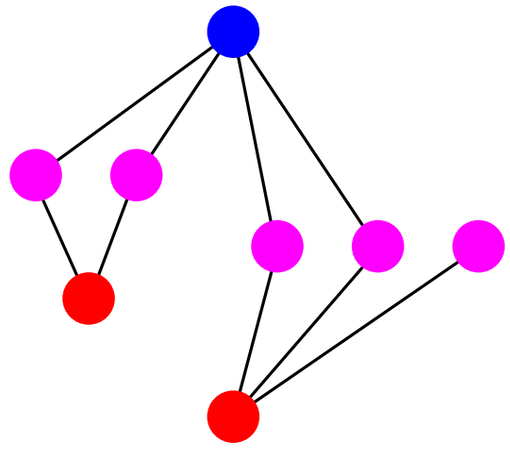


Structure of Mapper

Reminder: Mapper $\equiv$ *pixelized* Reeb graph







Structure of Mapper

Def: Given $X, f, \mathcal{I}$:

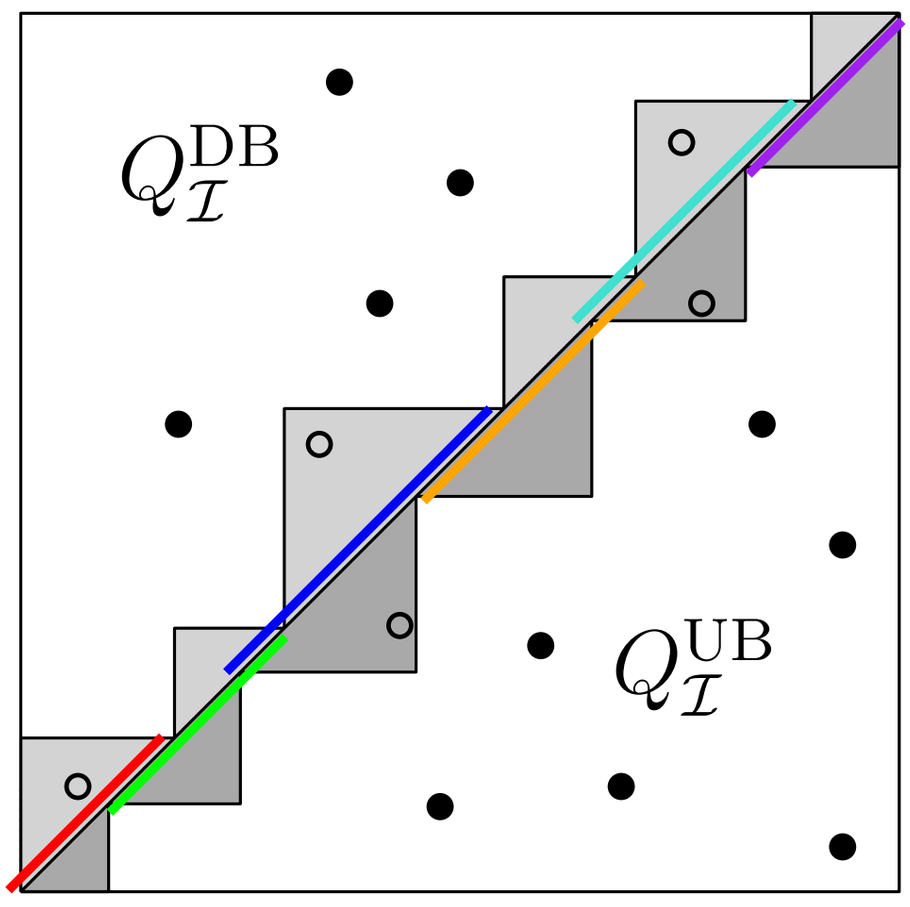
$$\mathrm{Dg}\left(\mathrm{M}_f\right) = \left(\mathrm{DB}(\mathrm{R}_f) \setminus Q_{\mathcal{I}}^{\mathrm{DB}}\right) \cup \left(\mathrm{UB}(\mathrm{R}_f) \setminus Q_{\mathcal{I}}^{\mathrm{UB}}\right) \cup \left(\mathrm{L}(\mathrm{R}_f) \setminus Q_{\mathcal{I}}^{\mathrm{L}}\right)$$

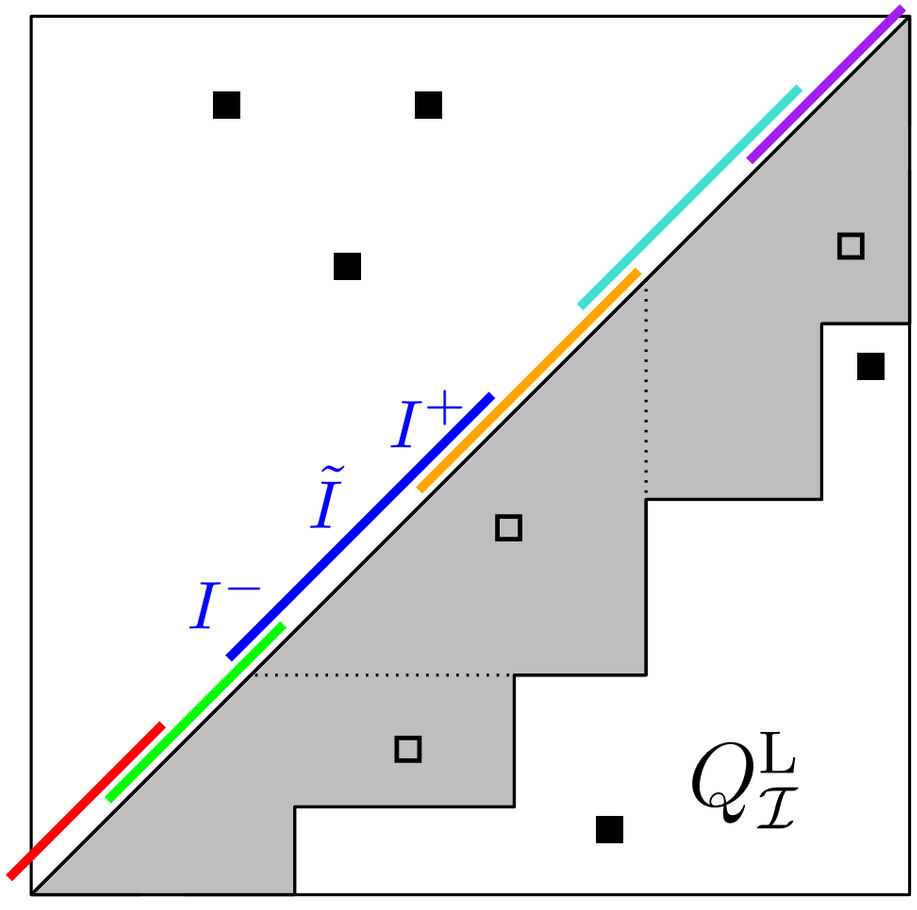
Structure of Mapper

Def: Given $X, f, \mathcal{I}$:

$$\mathrm{Dg}\left(\mathrm{M}_f\right) = \left(\mathrm{DB}(\mathrm{R}_f) \setminus Q_{\mathcal{I}}^{\mathrm{DB}}\right) \cup \left(\mathrm{UB}(\mathrm{R}_f) \setminus Q_{\mathcal{I}}^{\mathrm{UB}}\right) \cup \left(\mathrm{L}(\mathrm{R}_f) \setminus Q_{\mathcal{I}}^{\mathrm{L}}\right)$$

$$Q_{\mathcal{I}}^{\mathrm{DB}} = \bigcup_{I \in \mathcal{I}} Q^{+}_{\tilde{I} \cup I^{+}} \qquad Q_{\mathcal{I}}^{\mathrm{UB}} = \bigcup_{I \in \mathcal{I}} Q^{-}_{I^{-} \cup \tilde{I}} \qquad Q_{\mathcal{I}}^{\mathrm{L}} = \bigcup_{\substack{I, J \in \mathcal{I} \\ I \cap J \neq \emptyset}} Q^{-}_{I \cup J}$$





Structure of Mapper

Thm: [C., Oudot 2016]

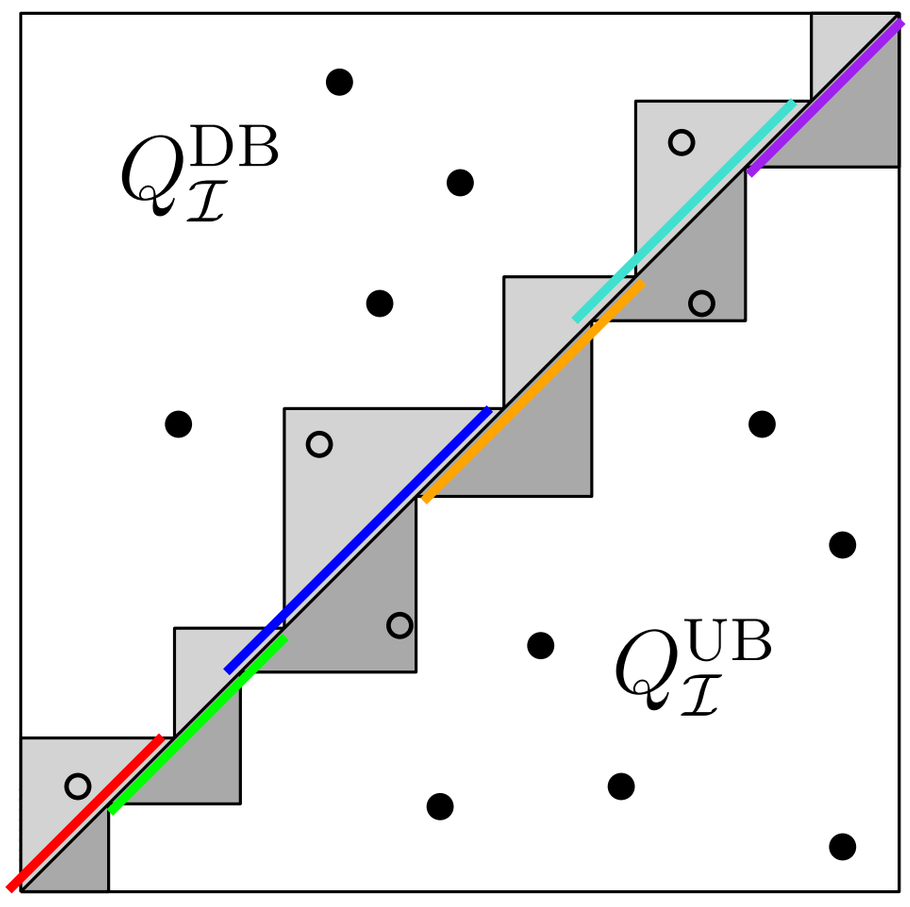
$\mathrm{Dg}\,(\mathrm{M}_f)$ provides a **bag-of-features** descriptor for $\mathrm{M}_f(X, \mathcal{I})$:

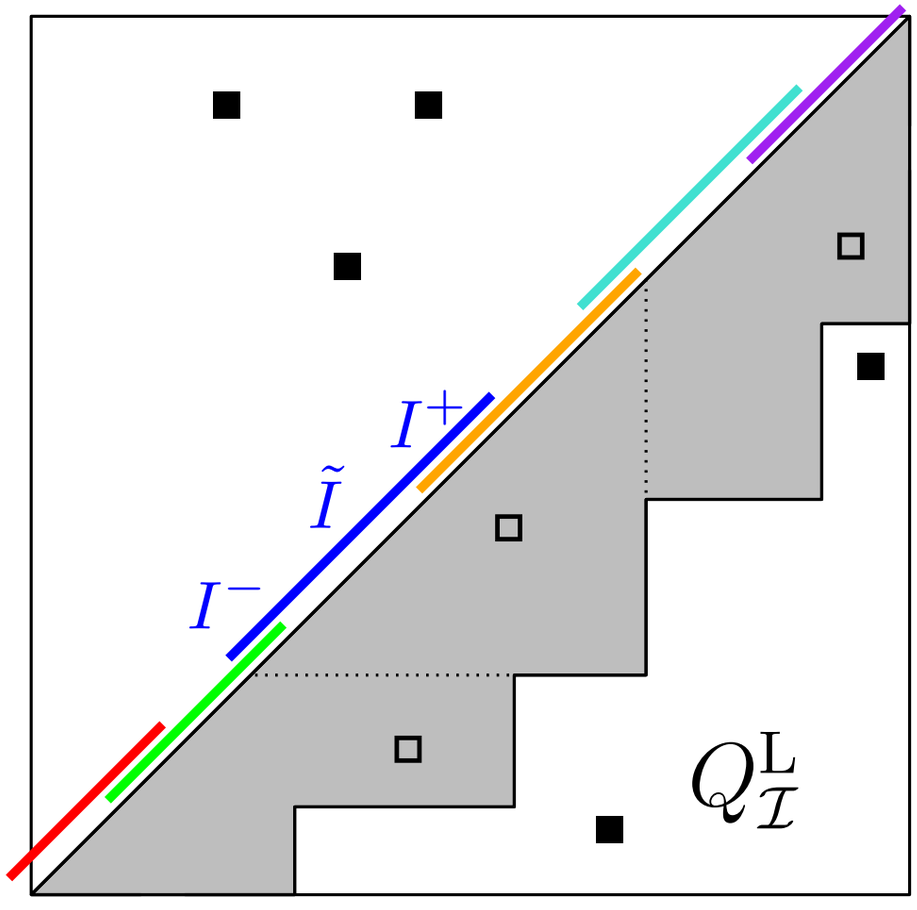
DB $\longleftrightarrow$ downward branches

UB $\longleftrightarrow$ upward branches

T $\longleftrightarrow$ trunks (cc)

L $\longleftrightarrow$ loops





Structure of Mapper

Thm: [C., Oudot 2016]

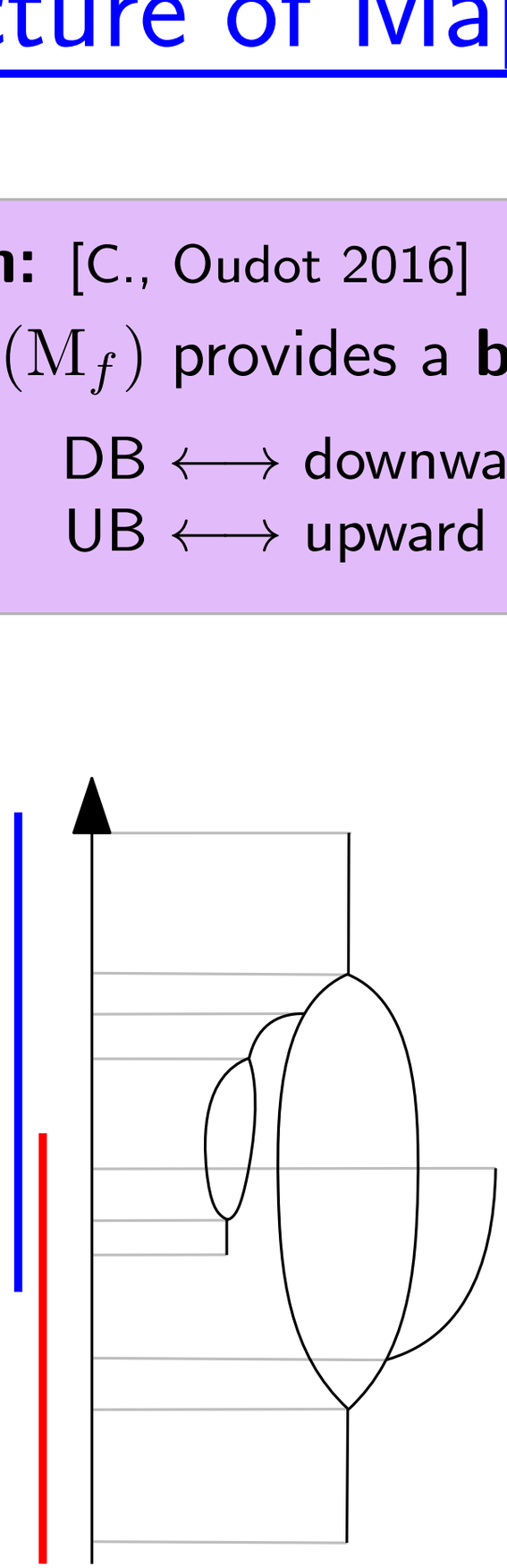
$\mathrm{Dg}\,(\mathrm{M}_f)$ provides a **bag-of-features** descriptor for $\mathrm{M}_f(X, \mathcal{I})$:

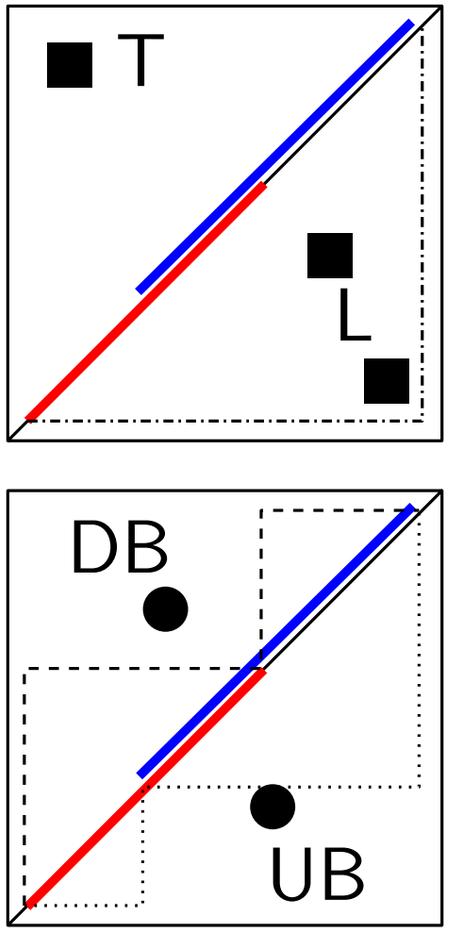
DB $\longleftrightarrow$ downward branches

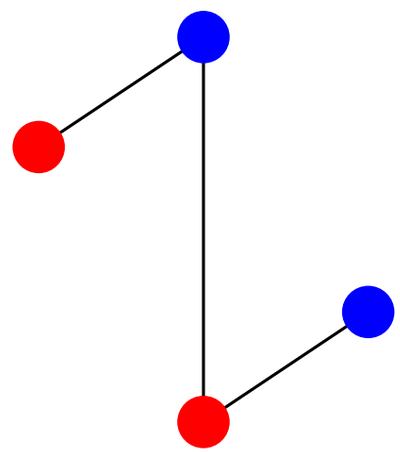
UB $\longleftrightarrow$ upward branches

T $\longleftrightarrow$ trunks (cc)

L $\longleftrightarrow$ loops







Structure of Mapper

Thm: [C., Oudot 2016]

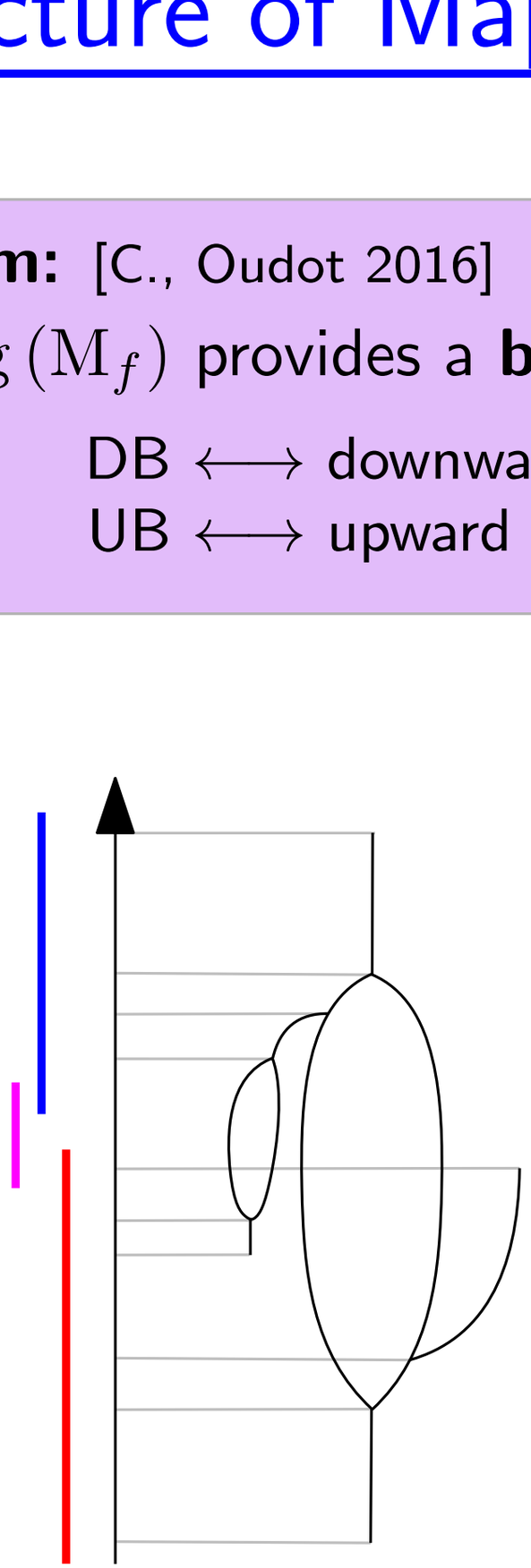
$\mathrm{Dg}\,(\mathrm{M}_f)$ provides a **bag-of-features** descriptor for $\mathrm{M}_f(X, \mathcal{I})$:

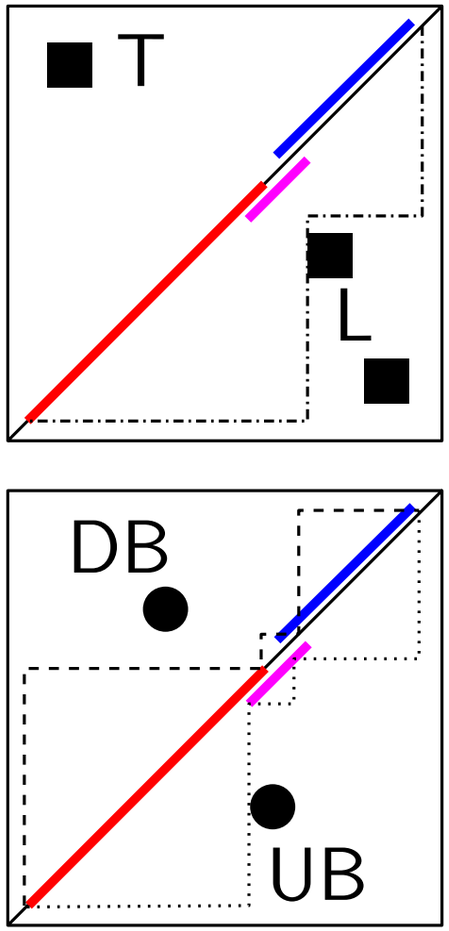
DB $\longleftrightarrow$ downward branches

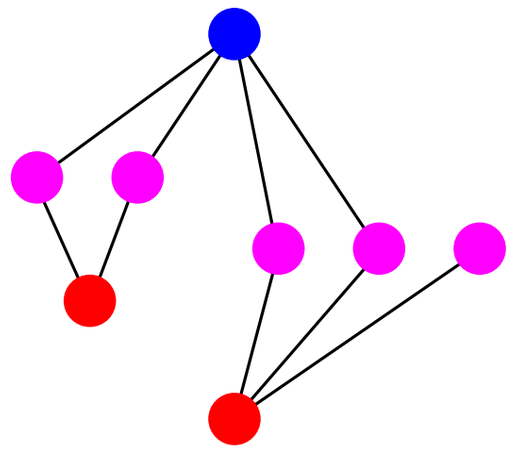
UB $\longleftrightarrow$ upward branches

T $\longleftrightarrow$ trunks (cc)

L $\longleftrightarrow$ loops

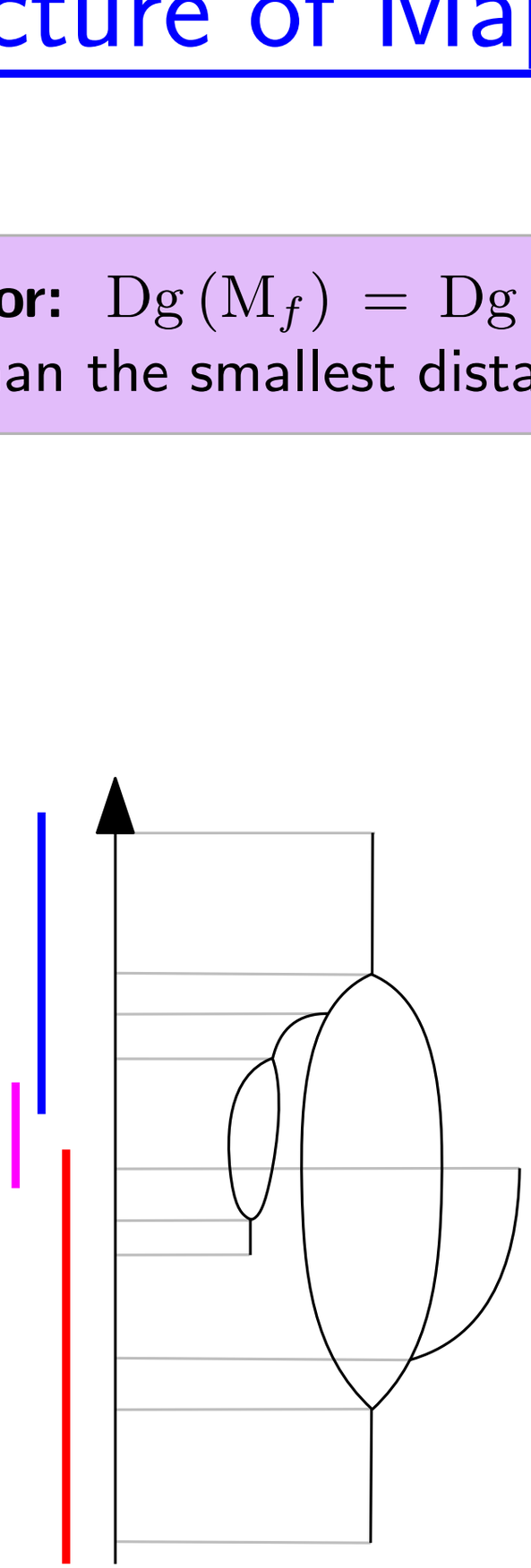


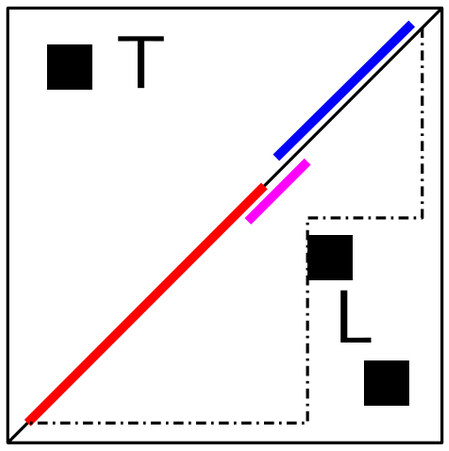


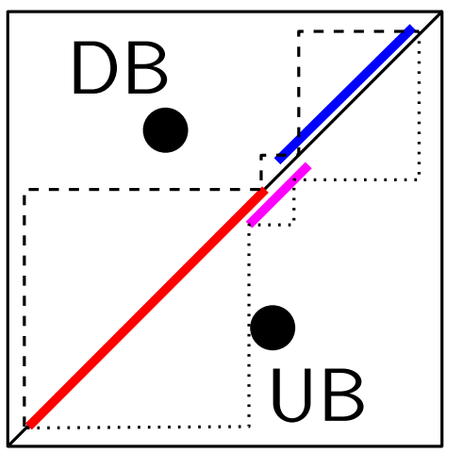


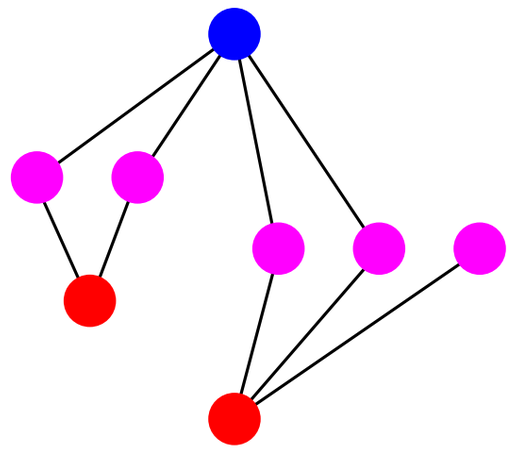
Structure of Mapper

Cor: $\mathrm{Dg}\left(\mathrm{M}_f\right) = \mathrm{Dg}\left(\mathrm{R}_f\right)$ whenever the resolution r of $\mathcal{I}$ is smaller than the smallest distance from $\mathrm{Dg}\left(\mathrm{R}_f\right) \setminus \Delta$ to the diagonal Δ





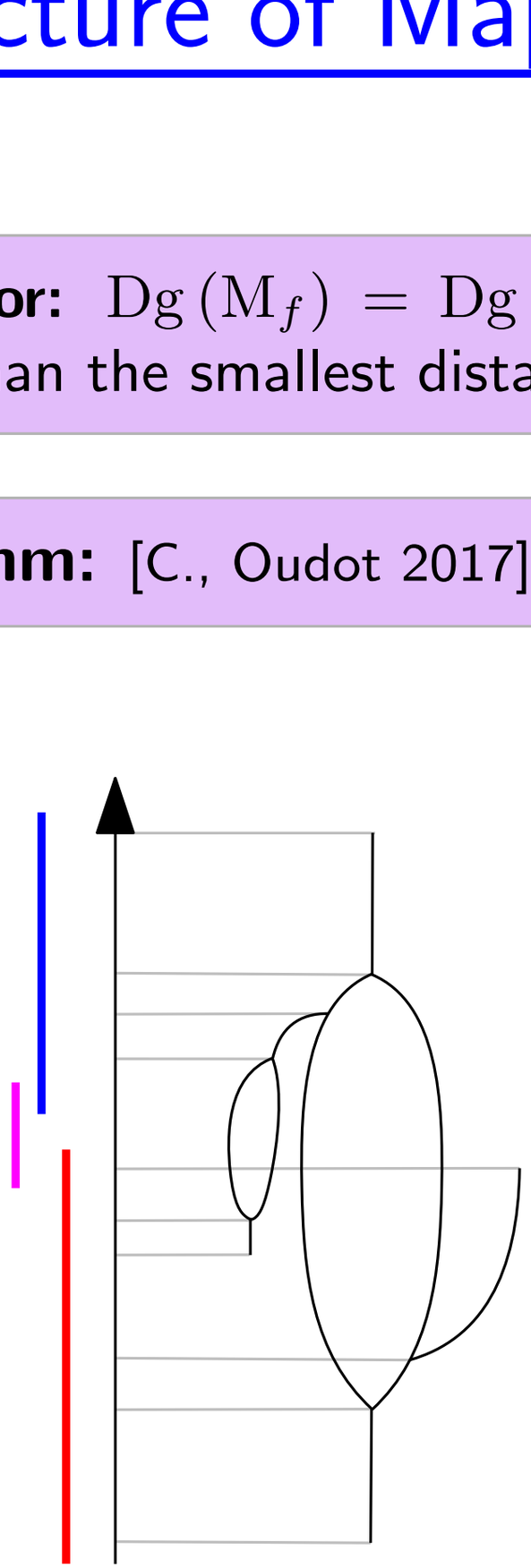


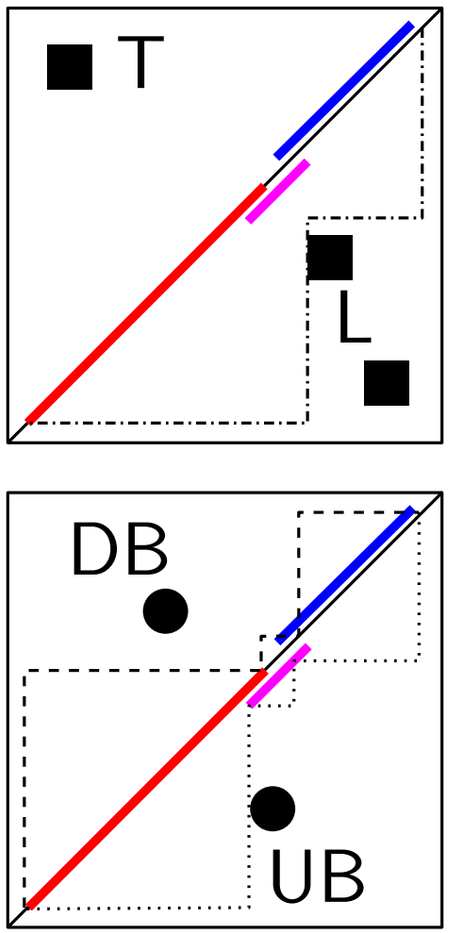


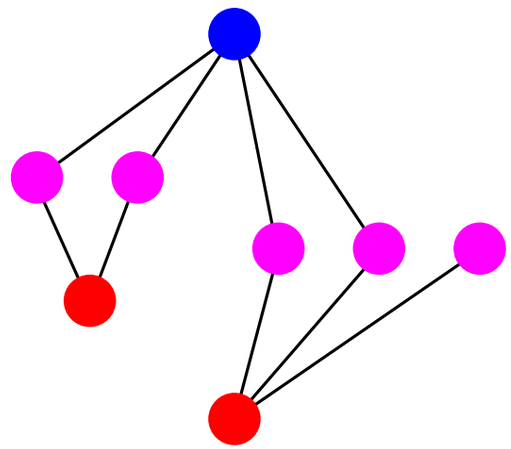
Structure of Mapper

Cor: $\mathrm{Dg}\,(\mathrm{M}_f) = \mathrm{Dg}\,(\mathrm{R}_f)$ whenever the resolution r of $\mathcal{I}$ is smaller than the smallest distance from $\mathrm{Dg}\,(\mathrm{R}_f) \setminus \Delta$ to the diagonal Δ

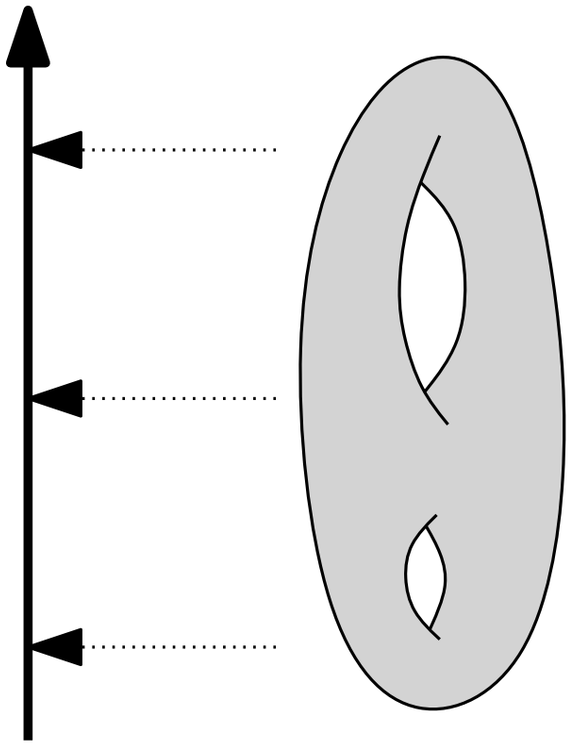
Thm: [C., Oudot 2017] $\mathrm{d_{GH}}(\mathrm{M}_f(X, \mathcal{I}), \mathrm{R}_f(X)) \leq 3r$

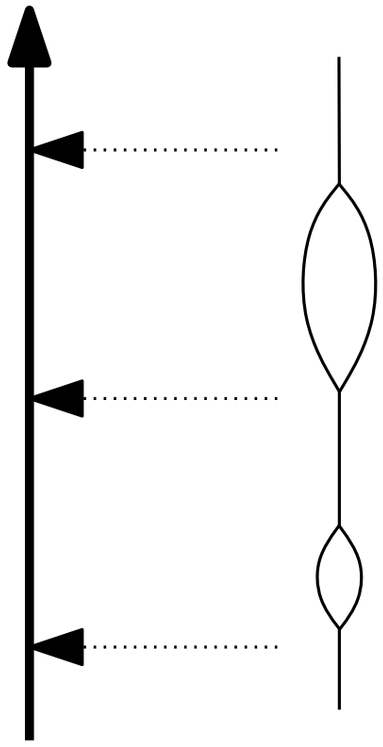


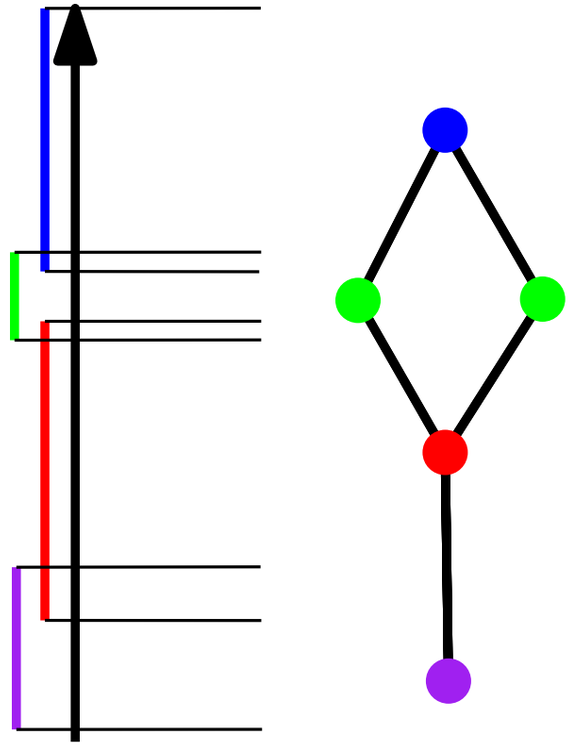


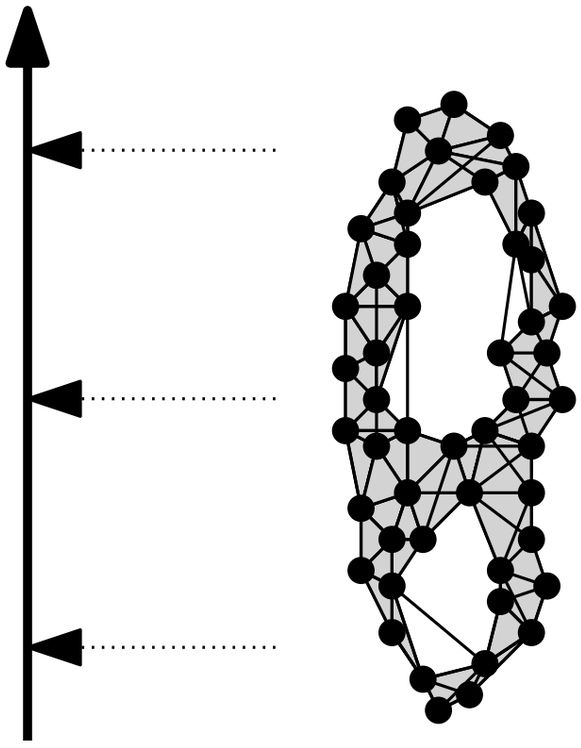


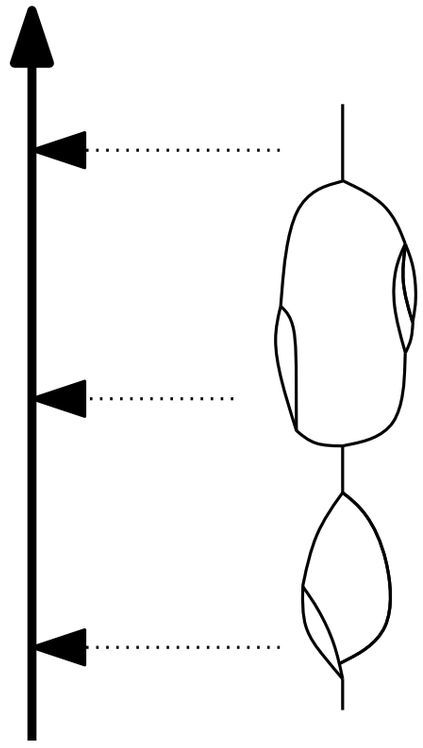
Statistics for Mapper

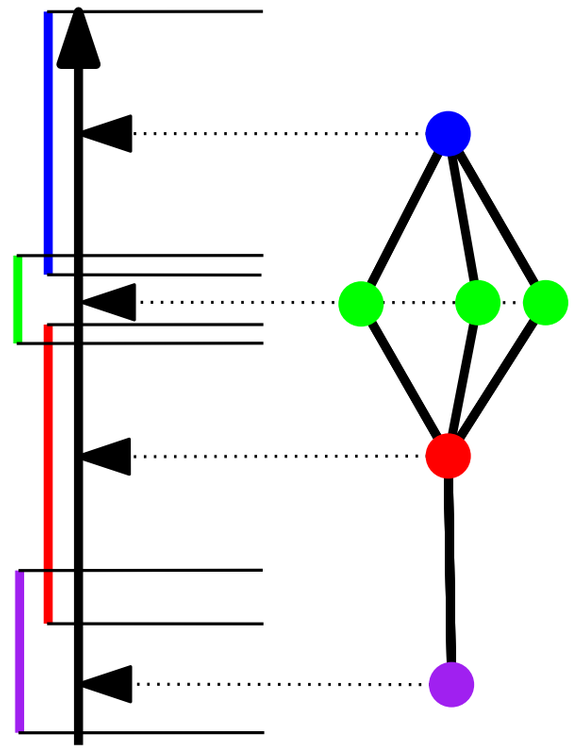




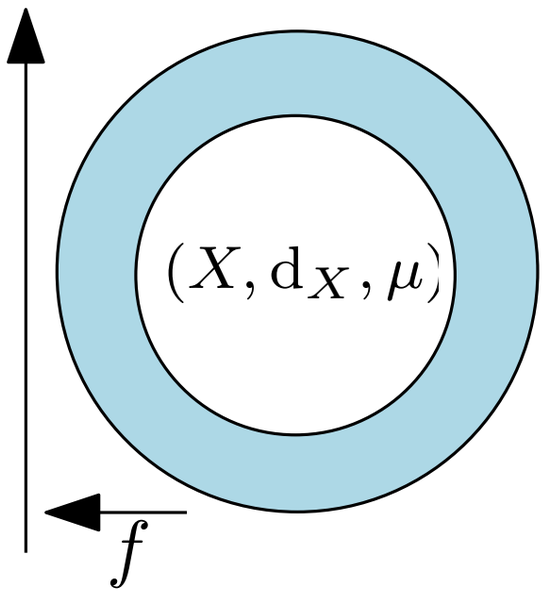




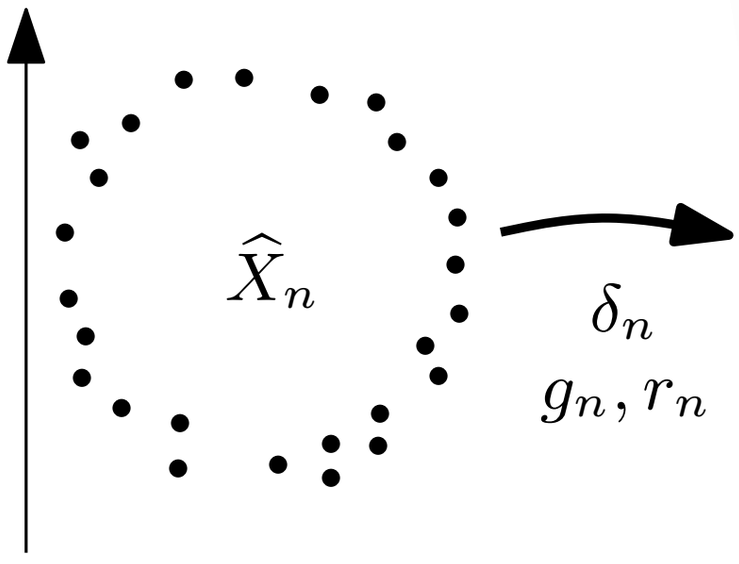


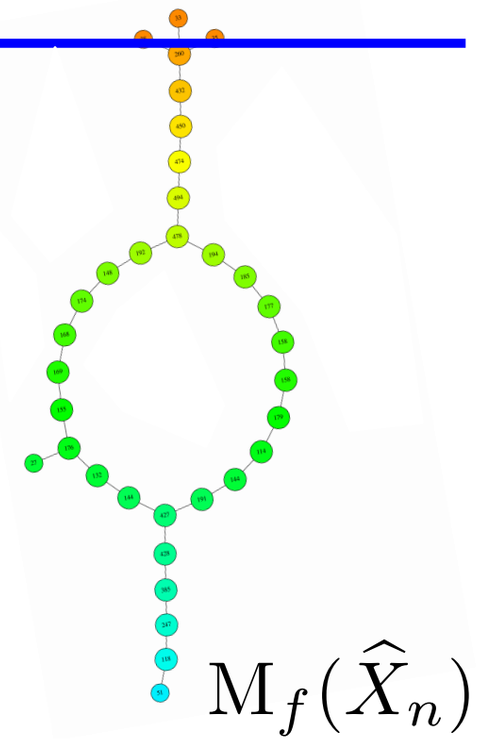


Setup

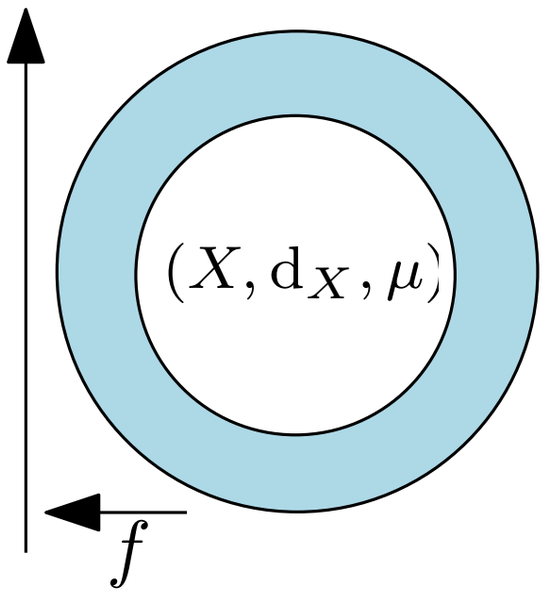


n points sampled
i.i.d. according to μ

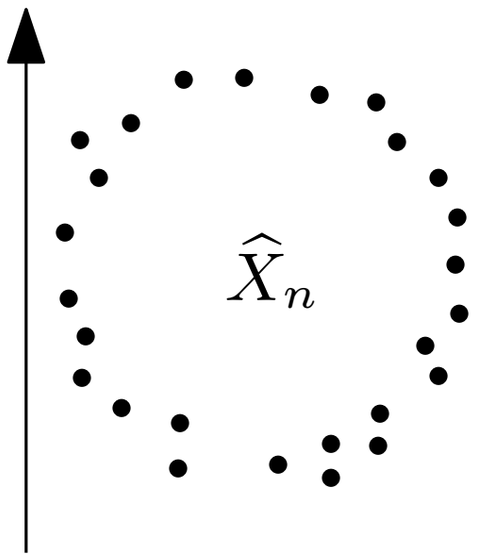




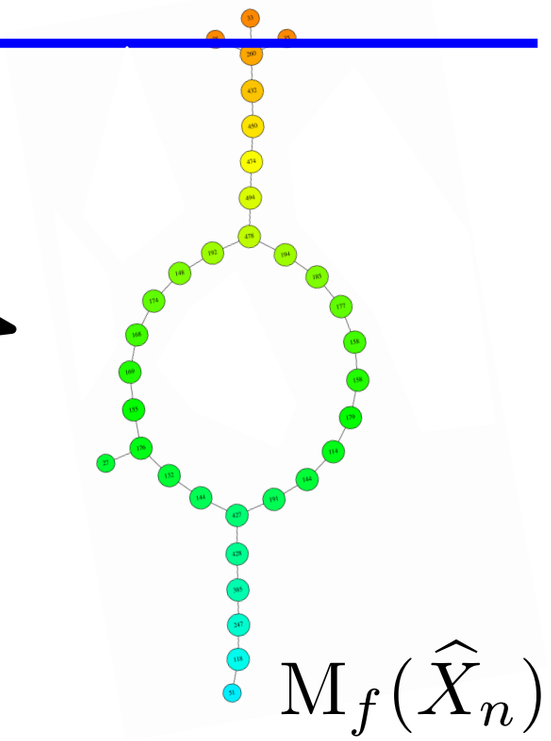
Setup



n points sampled
i.i.d. according to μ



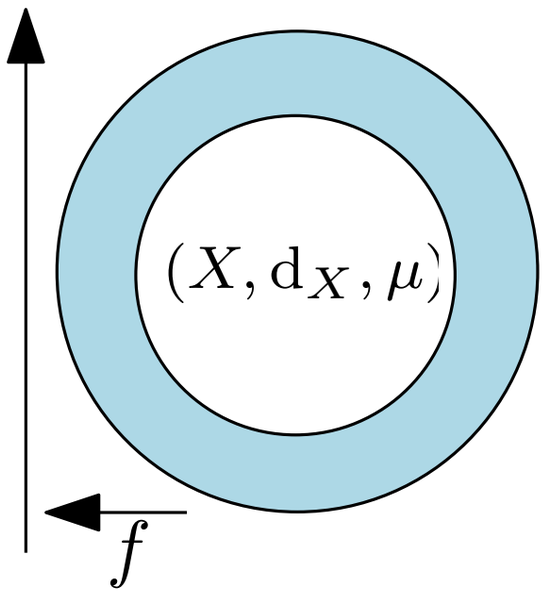
δ_n
g_n, r_n



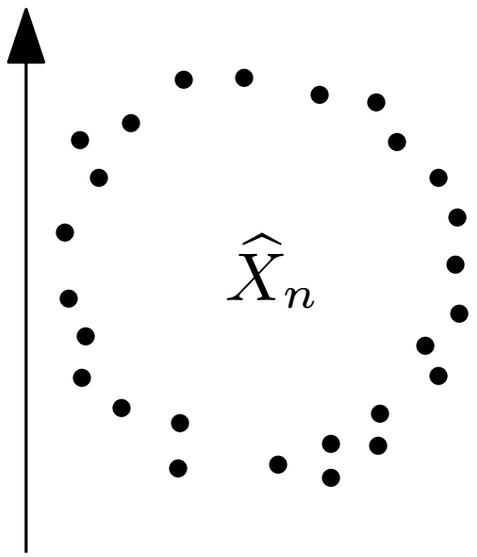
$\mathrm{M}_f(\widehat{X}_n)$

Prop: [C., Michel, Oudot 2017] $\widehat{\mathrm{M}}_n = \mathrm{M}_f(\widehat{X}_n)$ is measurable

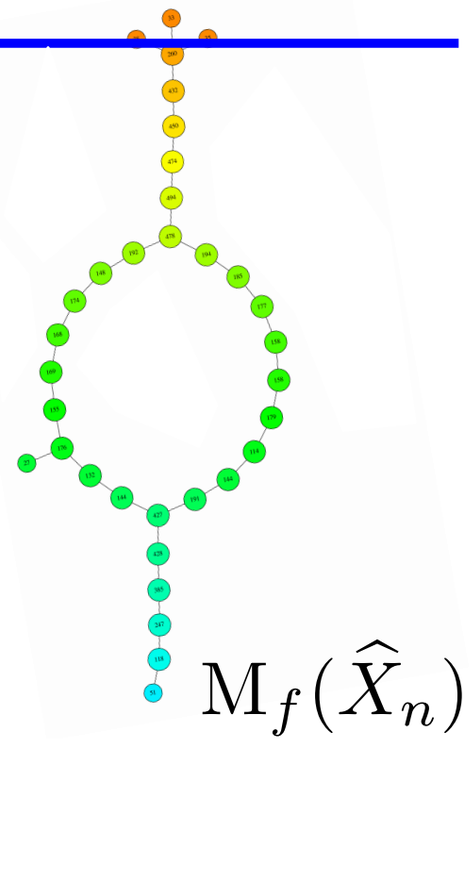
Setup



n points sampled
i.i.d. according to μ



δ_n
g_n, r_n

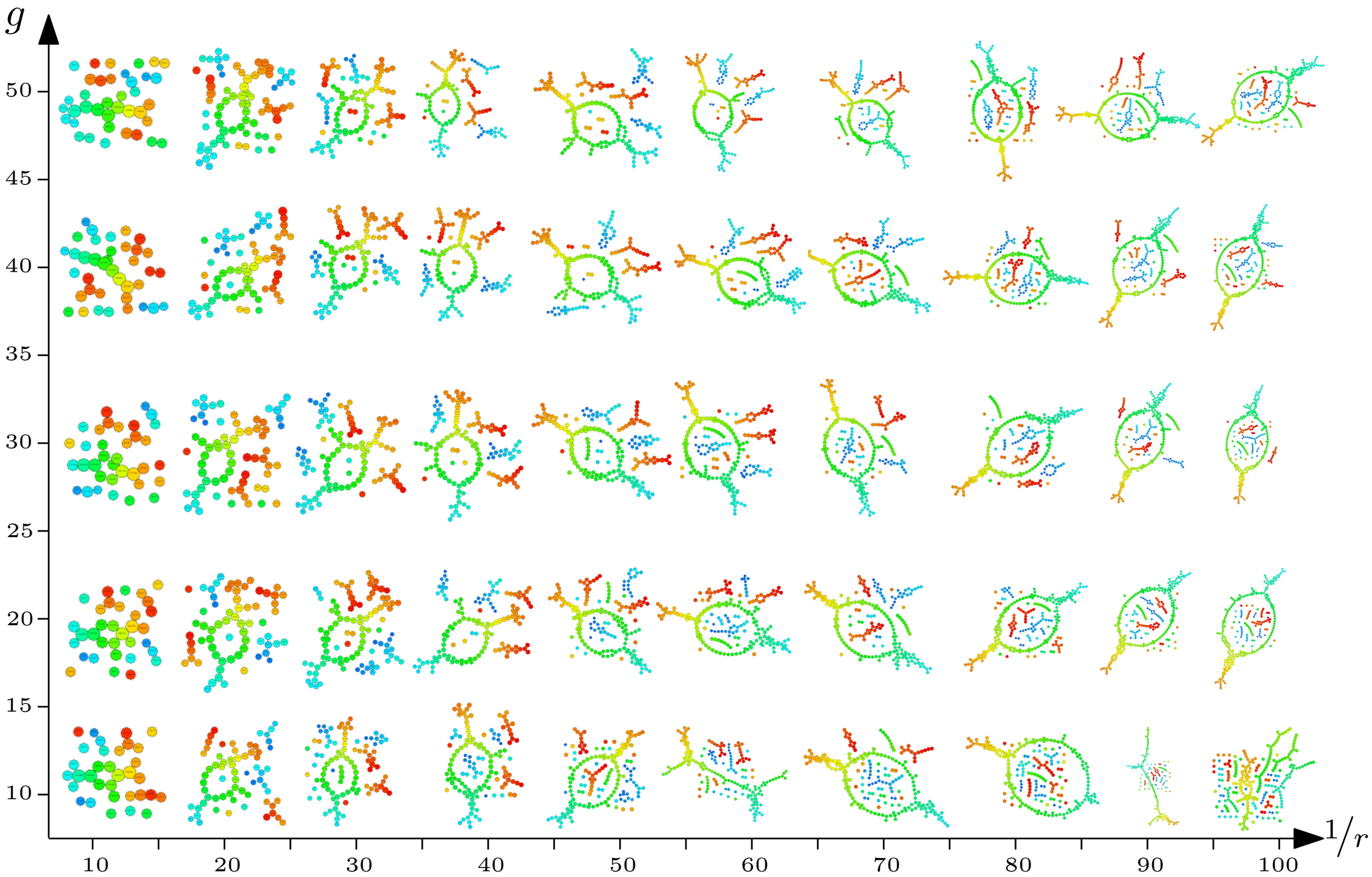


Prop: [C., Michel, Oudot 2017] $\widehat{\mathrm{M}}_n = \mathrm{M}_f(\widehat{X}_n)$ is measurable

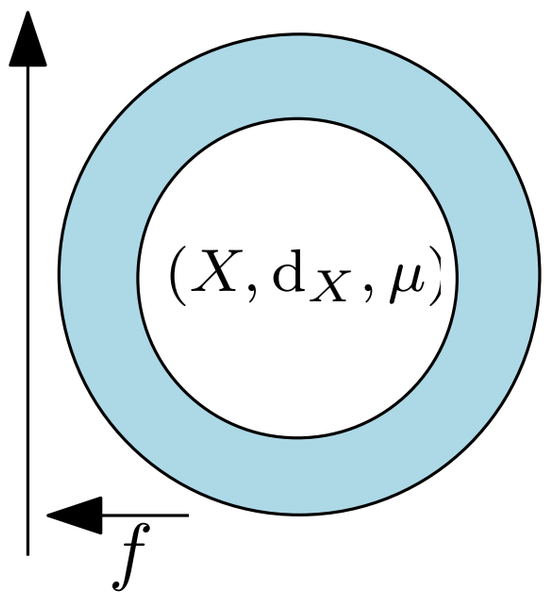
Goal: Find heuristics to compute "good" δ_n, g_n, r_n

Assess quality through confidence regions and convergence rates

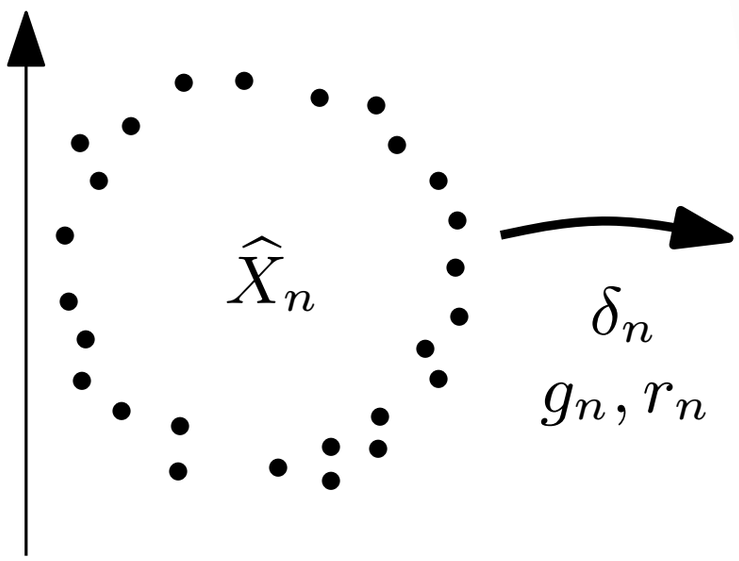
Setup

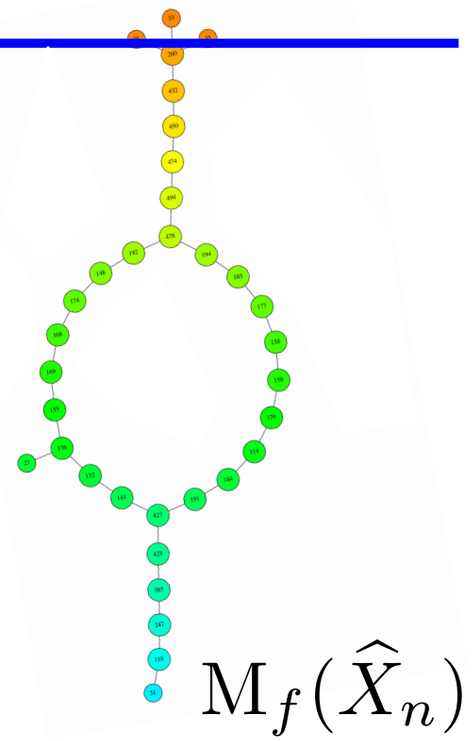


Setup



n points sampled
i.i.d. according to μ

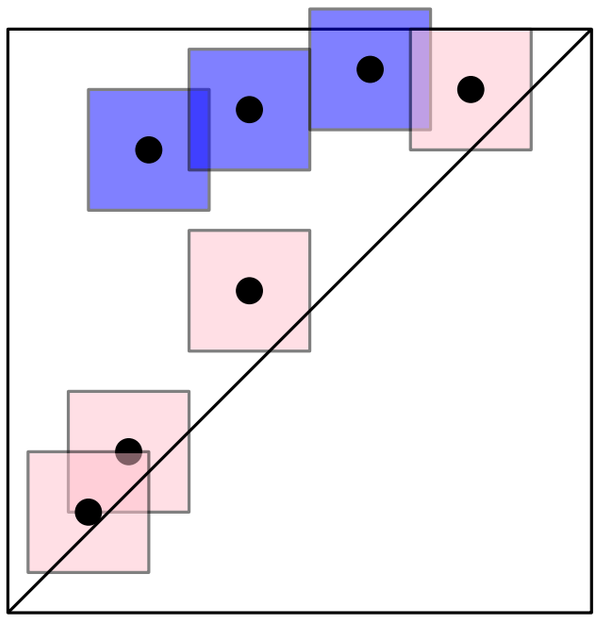


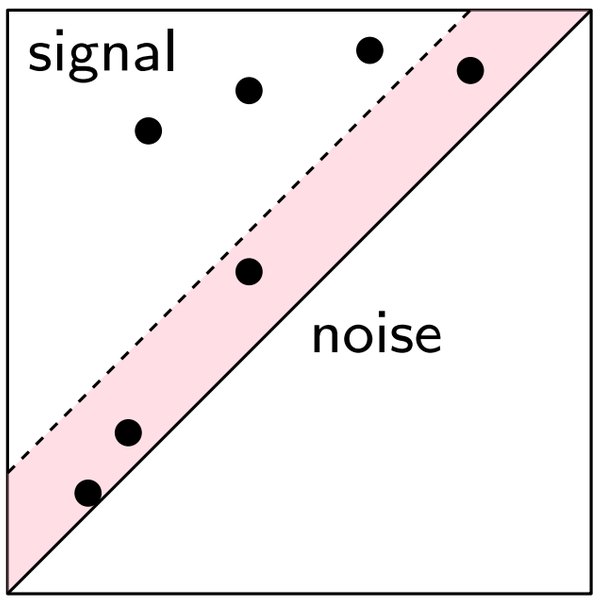


Confidence regions: given $\alpha \in (0,1)$, find $c_n(\alpha) \geq 0$ s.t.:

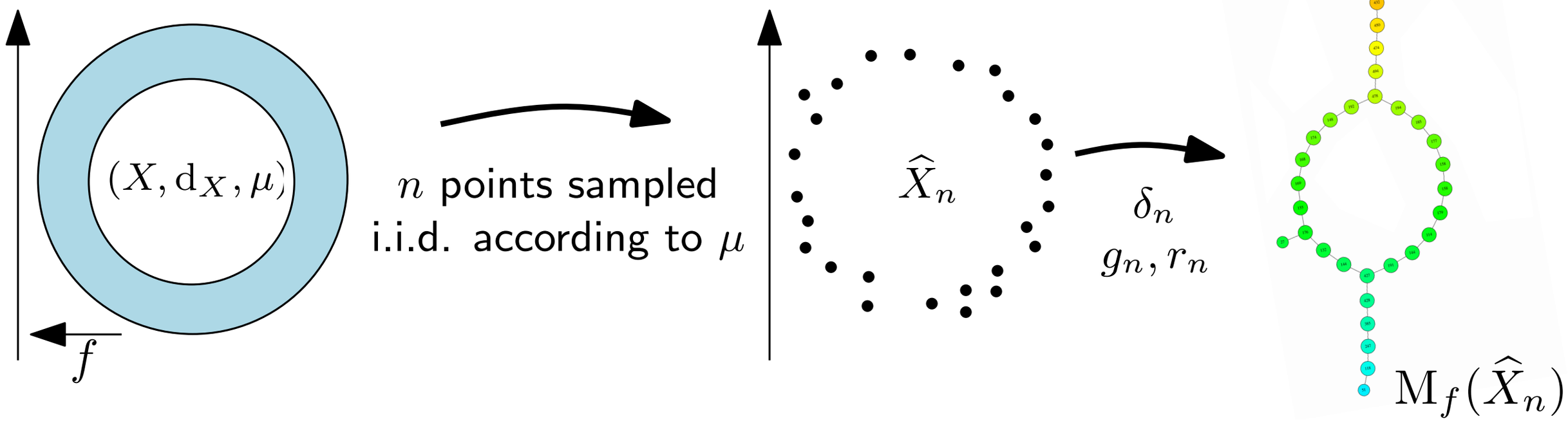
$$\limsup_{n\to\infty} \quad \mathbb{P}\left(\mathrm{d}_B\left(\widehat{\mathrm{M}}_n, \mathrm{R}_f(X)\right) > c_n(\alpha)\right) \leq \alpha$$

$\rightarrow$ d_B-ball of radius $c_n(\alpha)$ around $\mathrm{Dg}\left(\widehat{\mathrm{M}}_n\right)$





Setup



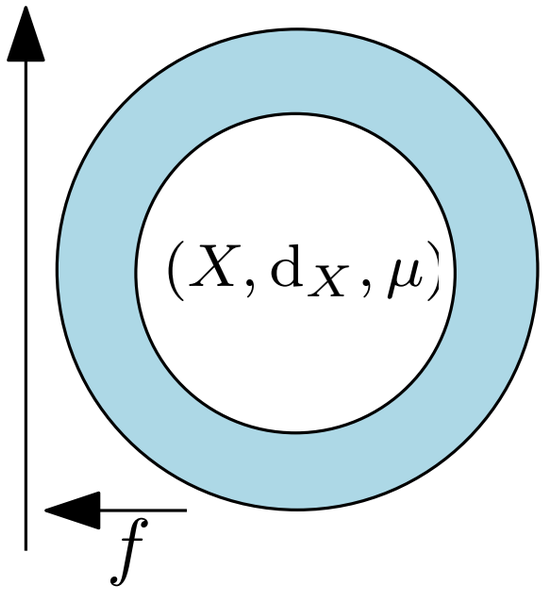
Confidence regions: given $\alpha \in (0,1)$, find $c_n(\alpha) \geq 0$ s.t.:

$$\limsup_{n\to\infty} \quad \mathbb{P}\left(\mathrm{d}_B\left(\widehat{\mathrm{M}}_n, \mathrm{R}_f(X)\right) > c_n(\alpha)\right) \leq \alpha$$

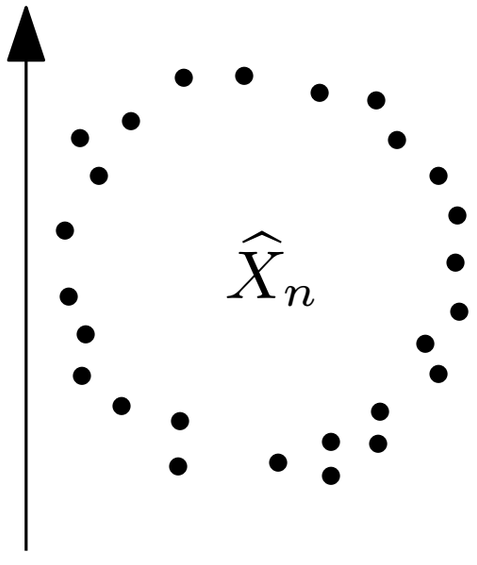
$\rightarrow$ d_B-ball of radius $c_n(\alpha)$ around $\mathrm{Dg}\left(\widehat{\mathrm{M}}_n\right)$

Convergence Rate: estimate $\mathbb{E}\left[\mathrm{d}_B(\widehat{\mathrm{M}}_n, \mathrm{R}_f(X))\right]$ w.r.t. n

Rate of Convergence

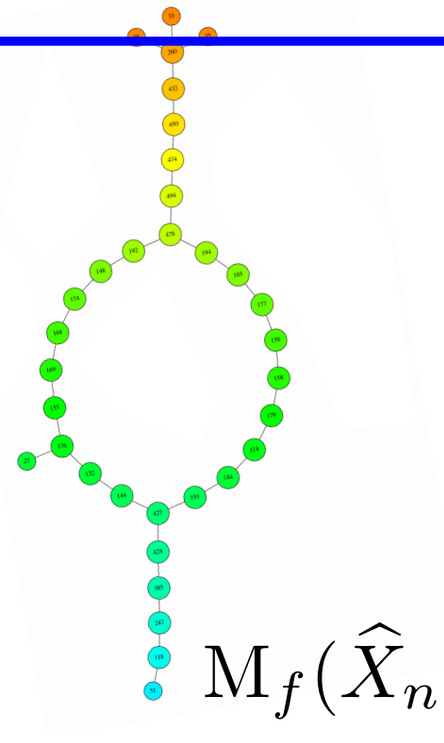


n points sampled
i.i.d. according to μ



δ_n

g_n, r_n



$\mathrm{M}_f(\widehat{X}_n)$

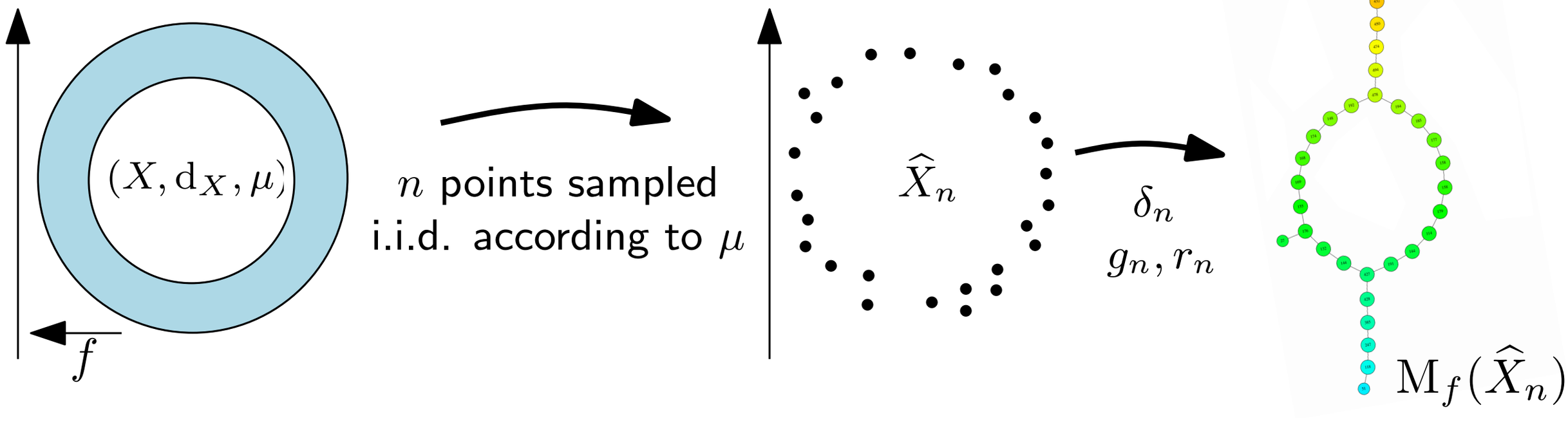
Regularity of the filter function: (exact) modulus of continuity of f

$$\omega(\delta) = \sup_{\|x-x'\| \leq \delta} |f(x) - f(x')|$$

Approximation inequality: [C., Michel, Oudot 2017]
Let $\widehat{X}_n \subset X$. Under some *regularity assumptions* on X, f, δ, r, g, one has:

$$\mathrm{d}_B \left(\mathrm{R}_f(X), \mathrm{M}_f(\widehat{X}_n) \right) \leq r + 2\omega(\delta)$$

Rate of Convergence



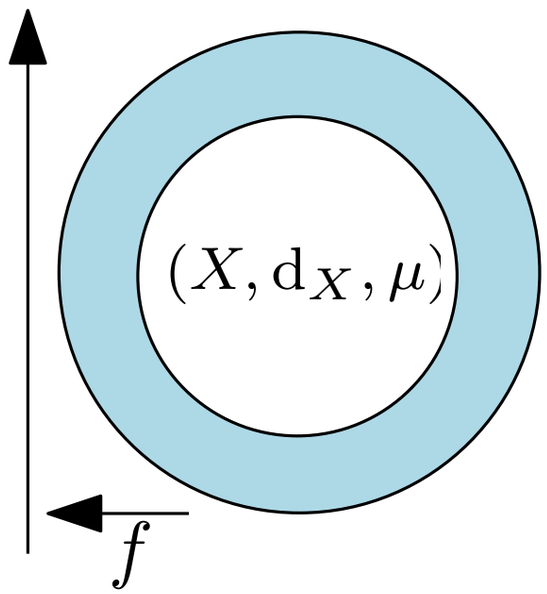
$$4\mathrm{d_H}(\widehat{X}_n, X) \leq \delta \leq C(X)$$

$$\max\{|f(X_i) - f(X_j)| \ : \ \|X_i - X_j\| \leq \delta\} < gr$$

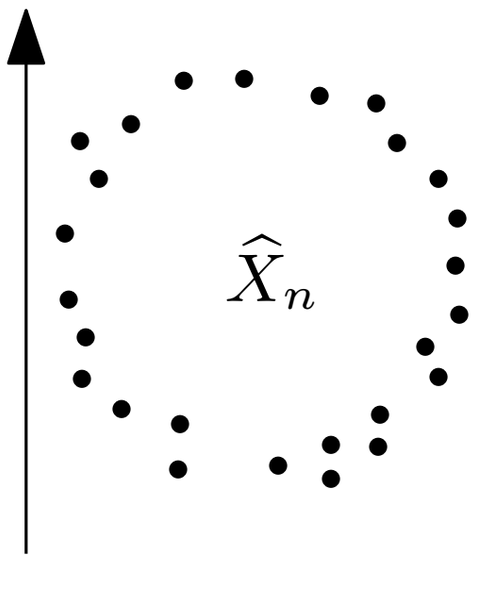
Approximation inequality: [C., Michel, Oudot 2017]
Let $\widehat{X}_n \subset X$. Under some *regularity assumptions* on X, f, δ, r, g, one has:

$$\mathrm{d}_B\left(\mathrm{R}_f(X), \mathrm{M}_f(\widehat{X}_n)\right) \leq r + 2\omega(\delta)$$

Rate of Convergence

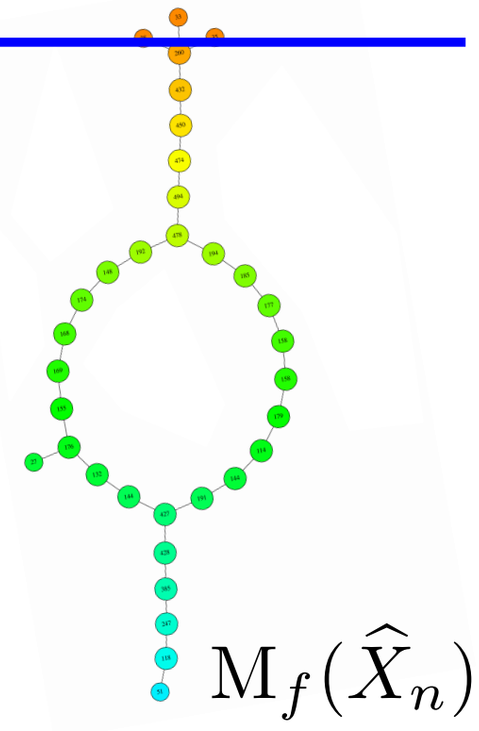


n points sampled
i.i.d. according to μ



δ_n

g_n, r_n



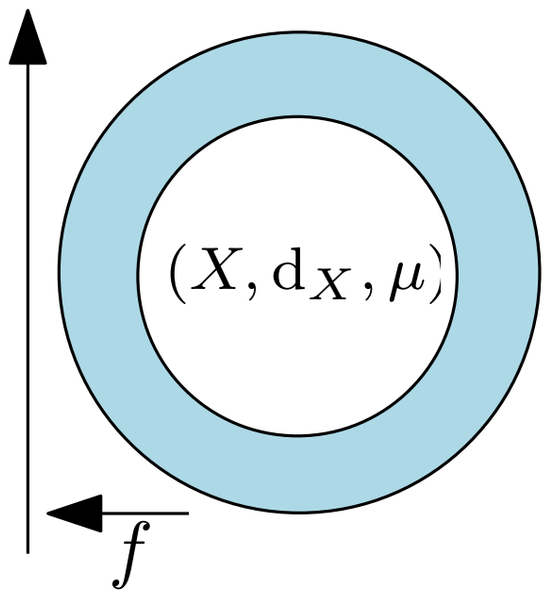
$$4\mathrm{d_H}(X_n, X) \leq \delta \leq C(X)$$

$$\max\{\max\{|f(X_i) - f(X_j)|, |\widehat{f}(X_i) - \widehat{f}(X_j)|\} \, : \, \|X_i - X_j\| \leq \delta\} \leq rg$$

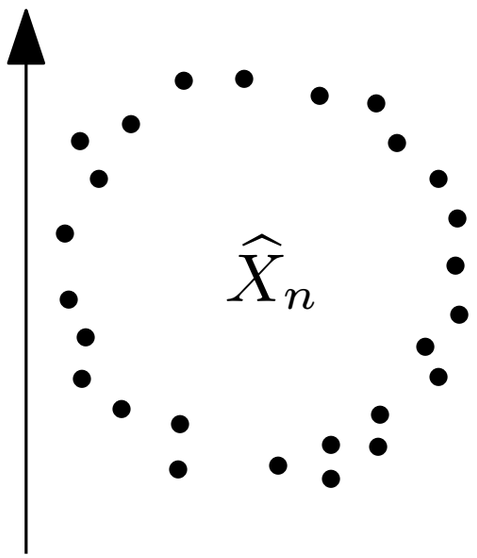
Approximation inequality: [C., Michel, Oudot 2017]
Let $\widehat{X}_n \subset X$. Under some *regularity assumptions* on X, f, δ, r, g, one has:

$$\mathrm{d}_B\left(\mathrm{R}_f(X), \mathrm{M}_{\widehat{f}}(\widehat{X}_n)\right) \leq 2r + 2\omega(\delta) + \max\{|f(X_i) - \widehat{f}(X_i)|\}$$

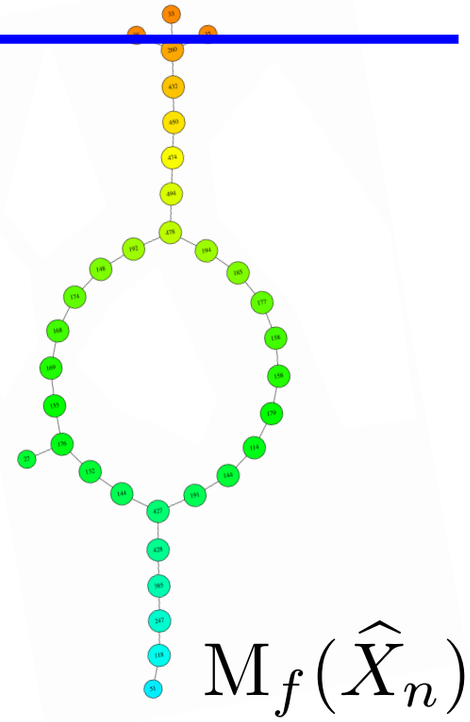
Rate of Convergence



n points sampled
i.i.d. according to μ



δ_n
g_n, r_n



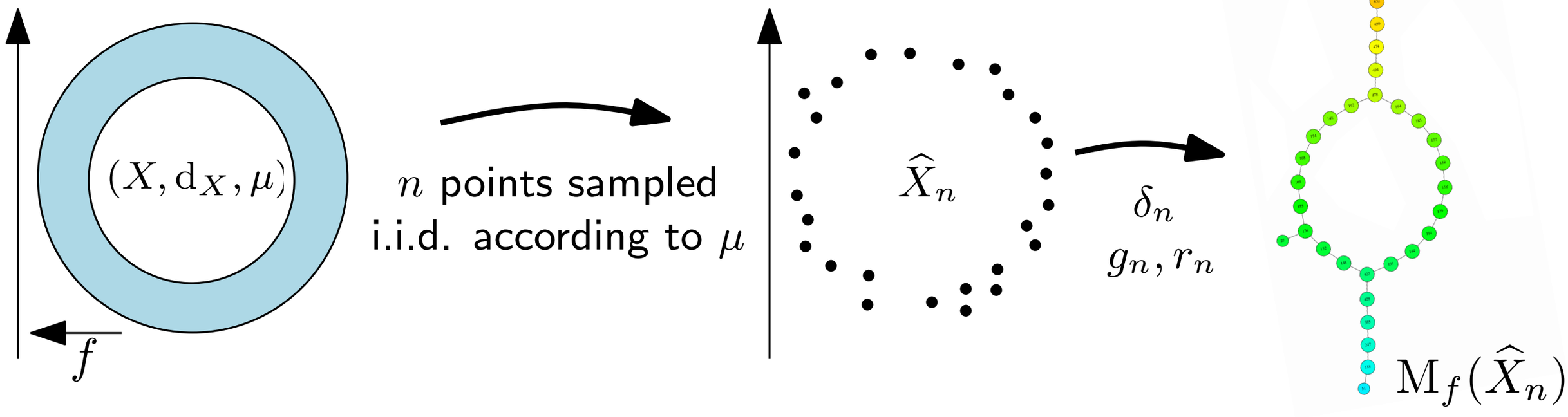
$$V_n = \max\{f(X_i) - f(X_j) \ : \ \|X_i - X_j\| \leq \delta_n\}$$

Thm: [C., Michel, Oudot 2017]

If μ is (a, b)-standard, then for $\delta_n = 4\left(\frac{2\log n}{an}\right)^{1/b}$, $g_n \in \left(\frac{1}{3}, \frac{1}{2}\right)$, $r_n = \frac{V_n}{g_n}$, one has:

$$\sup_{\mu \in \mathcal{P}} \mathbb{E}\left[\mathrm{d}_B\left(\mathrm{M}_f(\widehat{X}_n), \mathrm{R}_f(X)\right)\right] \lesssim \omega\left(\frac{\log n}{n}\right)^{1/b}$$

Rate of Convergence



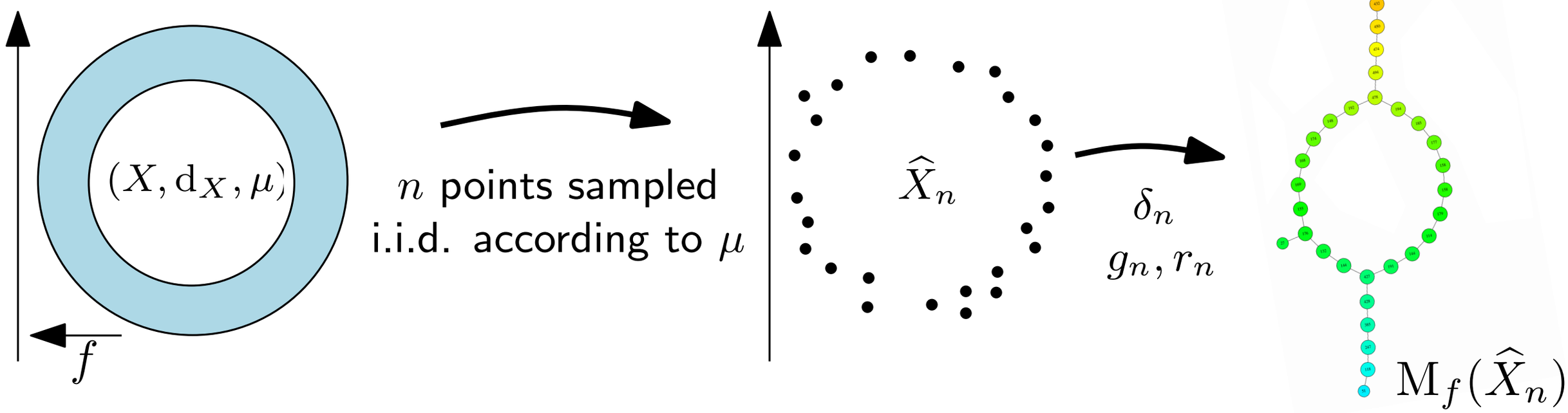
$$V_n = \max\{f(X_i) - f(X_j) \ : \ \|X_i - X_j\| \leq \delta_n\}$$

Thm: [C., Michel, Oudot 2017]

If μ is (a, b)-standard, then for $\delta_n = 4\left(\frac{2\log n}{an}\right)^{1/b}$, $g_n \in \left(\frac{1}{3}, \frac{1}{2}\right)$, $r_n = \frac{V_n}{g_n}$, one has:

$$\sup_{\mu \in \mathcal{P}} \mathbb{E}\left[\mathrm{d}_B\left(\mathrm{M}_f(\widehat{X}_n), \mathrm{R}_f(X)\right)\right] \lesssim \omega\left(\frac{\log n}{n}\right)^{1/b}$$

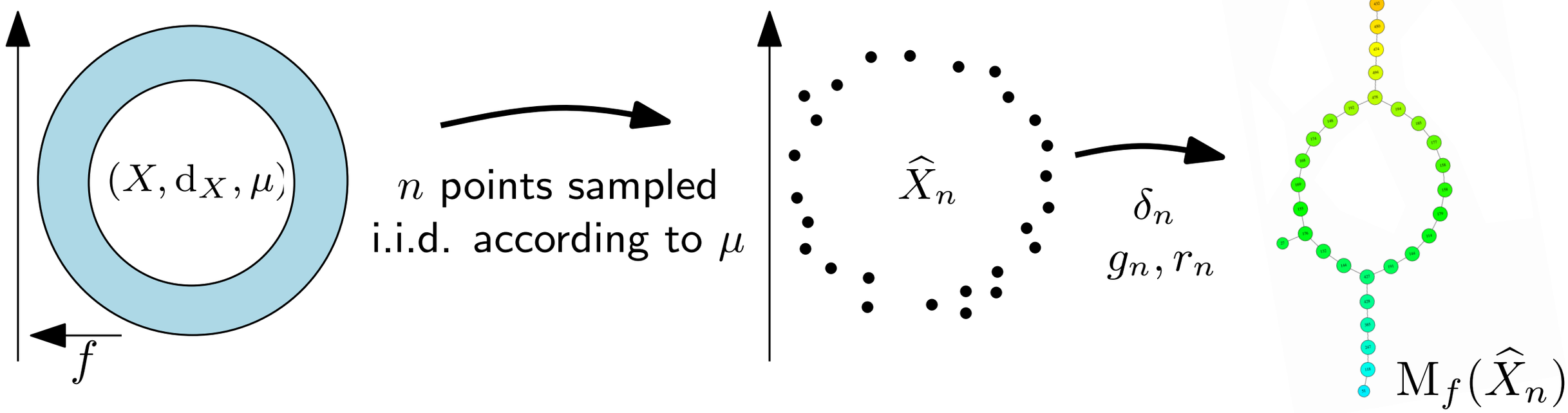
Rate of Convergence



Subsampling to tune δ_n: let $\beta > 0$ and take $s(n) = n\log(n)^{-(1+\beta)}$

$\delta_n = \mathrm{d_H}(\hat{X}_n^{s(n)}, \hat{X}_n)$ where $\hat{X}_n^{s(n)} \subset \hat{X}_n$ of size $s(n)$

Rate of Convergence



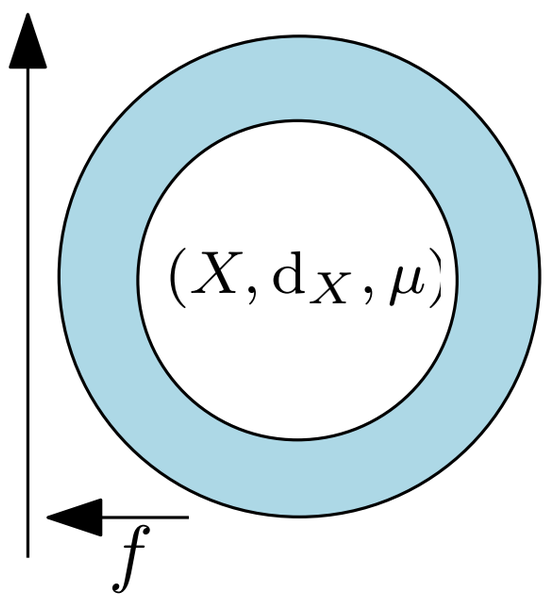
Subsampling to tune δ_n: let $\beta > 0$ and take $s(n) = n\log(n)^{-(1+\beta)}$

$\delta_n = \mathrm{d_H}(\hat{X}_n^{s(n)}, \hat{X}_n)$ where $\hat{X}_n^{s(n)} \subset \hat{X}_n$ of size $s(n)$

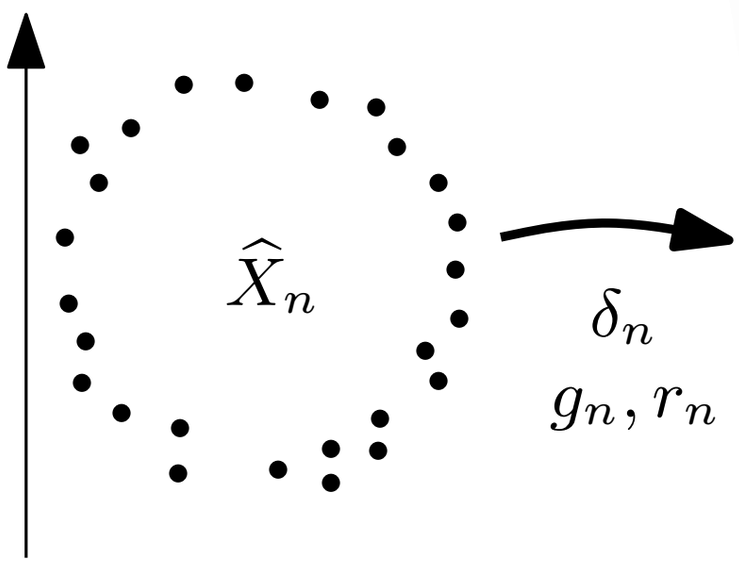
Thm: [C., Michel, Oudot 2017]
If μ is (a, b)-standard, then for δ_n, $g_n \in \left(\frac{1}{3}, \frac{1}{2}\right)$, $r_n = \frac{V_n}{g_n}$, one has

$$\sup_{\mu \in \mathcal{P}} \mathbb{E}\left[\mathrm{d}_B\left(\mathrm{M}_f(\widehat{X}_n), \mathrm{R}_f(X)\right)\right] \lesssim \omega\left(\frac{\log(n)^{2+\beta}}{n}\right)^{1/b}$$

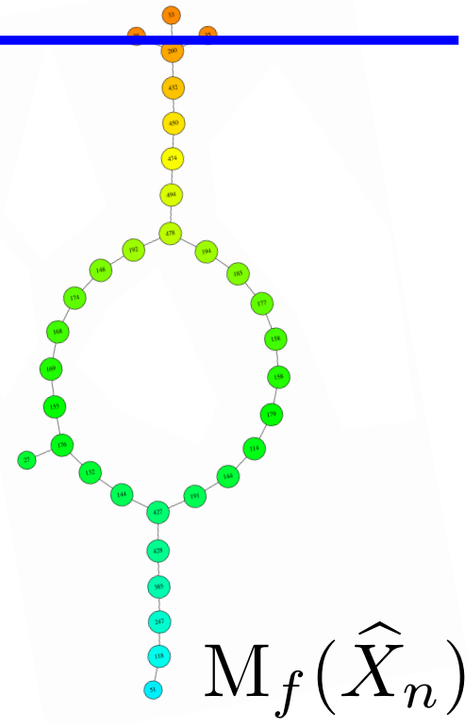
Rate of Convergence



n points sampled
i.i.d. according to μ



δ_n
g_n, r_n



Subsampling to tune δ_n: let $\beta > 0$ and take $s(n) = n\log(n)^{-(1+\beta)}$

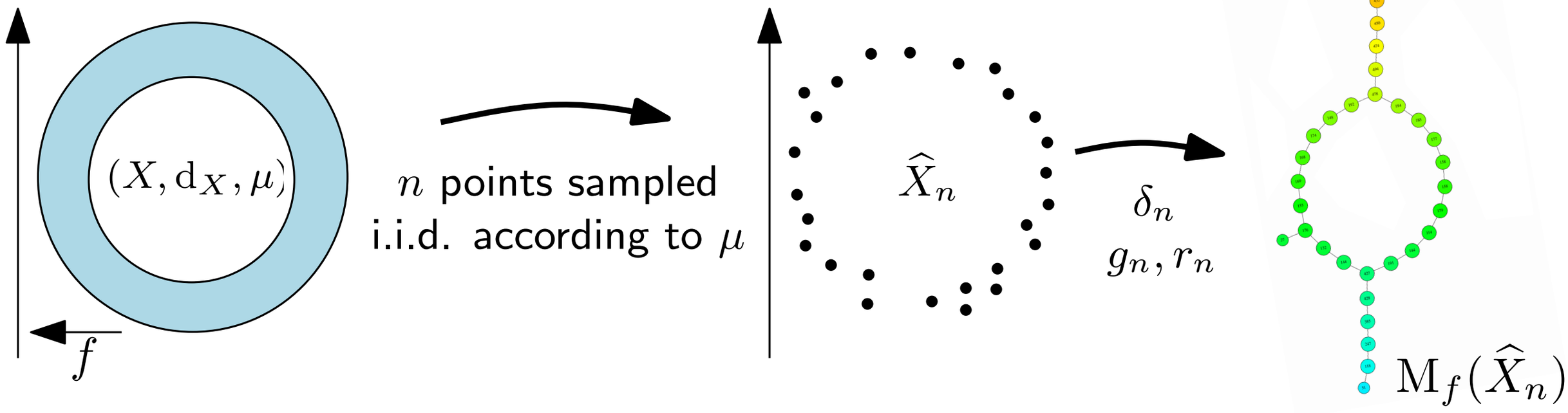
$\delta_n = \mathrm{d_H}(\hat{X}_n^{s(n)}, \hat{X}_n)$ where $\hat{X}_n^{s(n)} \subset \hat{X}_n$ of size $s(n)$

Thm: [C., Michel, Oudot 2017]

If μ is (a, b)-standard, then for δ_n, $g_n \in \left(\frac{1}{3}, \frac{1}{2}\right)$, $r_n = \frac{\max\{V_n, \widehat{V}_n\}}{g_n}$, one has

$$\sup_{\mu \in \mathcal{P}} \mathbb{E}\left[\mathrm{d}_B\left(\mathrm{M}_{\widehat{f}}(\widehat{X}_n), \mathrm{R}_f(X)\right)\right] \lesssim \omega\left(\frac{\log(n)^{2+\beta}}{n}\right)^{1/b} + \mathbb{E}\left[\max|f(X) - \widehat{f}(X)|\right]$$

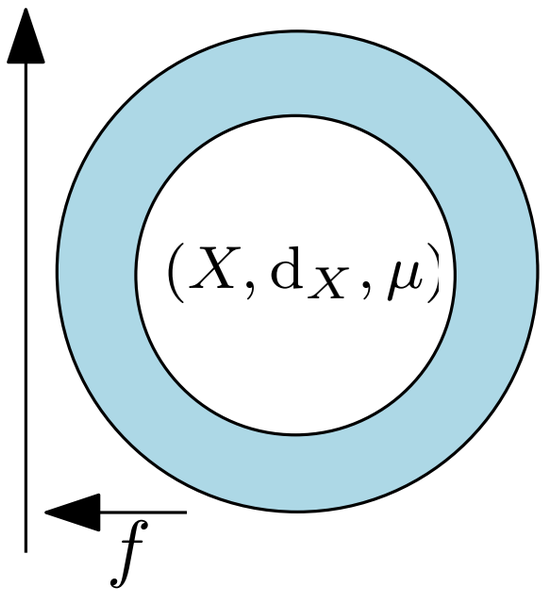
Rate of Convergence



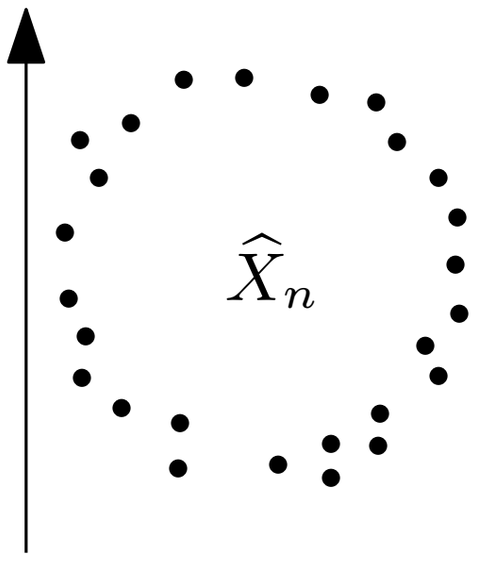
Minimax Optimality: [C., Michel, Oudot 2017] for any estimator $\widehat{\mathrm{R}}_n$,

$$\omega\left(\frac{1}{n}\right)^{1/b} \lesssim \sup_{\mu \in \mathcal{P}} \mathbb{E}\left[\mathrm{d}_B\left(\widehat{\mathrm{R}}_n, \mathrm{R}_f(X)\right)\right]$$

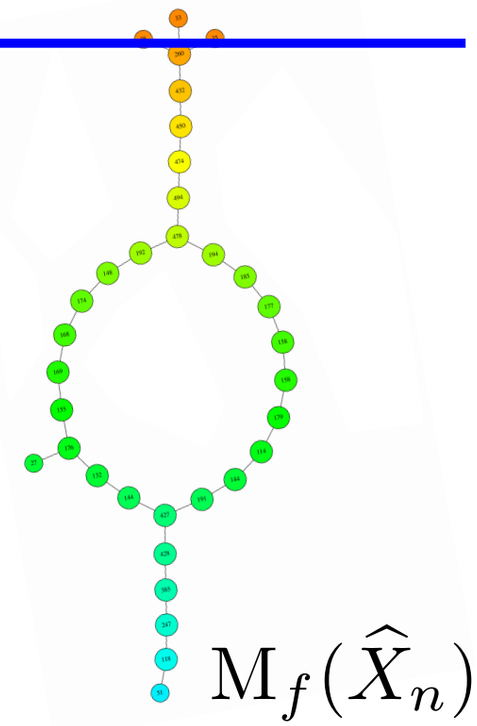
Rate of Convergence



n points sampled
i.i.d. according to μ



δ_n
g_n, r_n



Ex : PCA filter

Π_1: 1st principal direction of covariance operator
$\widehat{\Pi}_1$: 1st principal direction of empirical covariance operator
Using [Biau et. al. 2012]:

$$\mathbb{E}\left[\mathrm{d}_B\left(\mathrm{R}_{\Pi_1}(X), \mathrm{M}_{\widehat{\Pi}_1}(\widehat{X}_n)\right)\right] \lesssim \left(\frac{\log(n)^{2+\beta}}{n}\right)^{1/b} \vee \frac{1}{\sqrt{n}}$$

Confidence Regions

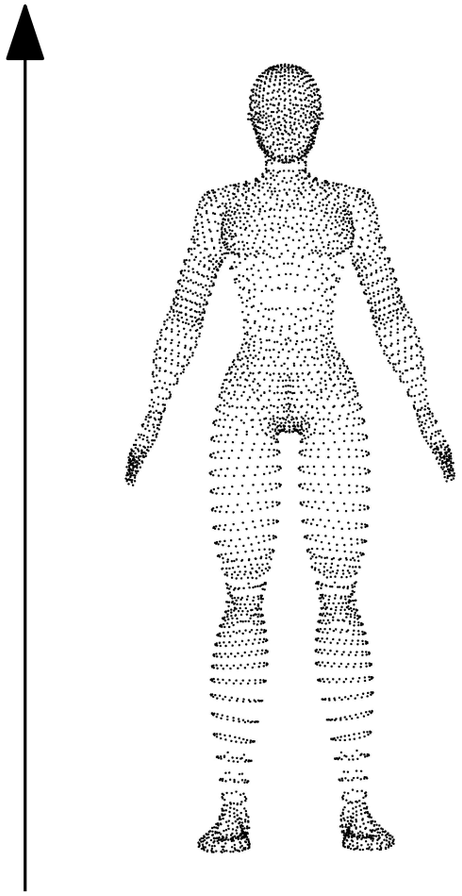
Either from proof of previous result with:

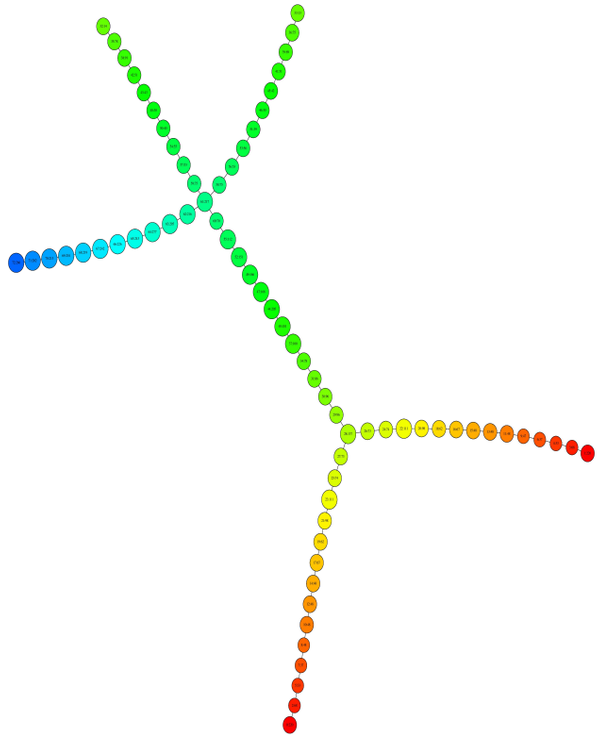
$$\mathbb{E}\left[\mathrm{d}_B\left(\mathrm{M}_f(\widehat{X}_n), \mathrm{R}_f(X)\right)\right] = \int_\alpha \mathbb{P}\left(\mathrm{d}_B\left(\mathrm{M}_f(\widehat{X}_n), \mathrm{R}_f(X)\right) \geq \alpha\right) \mathrm{d}\alpha$$

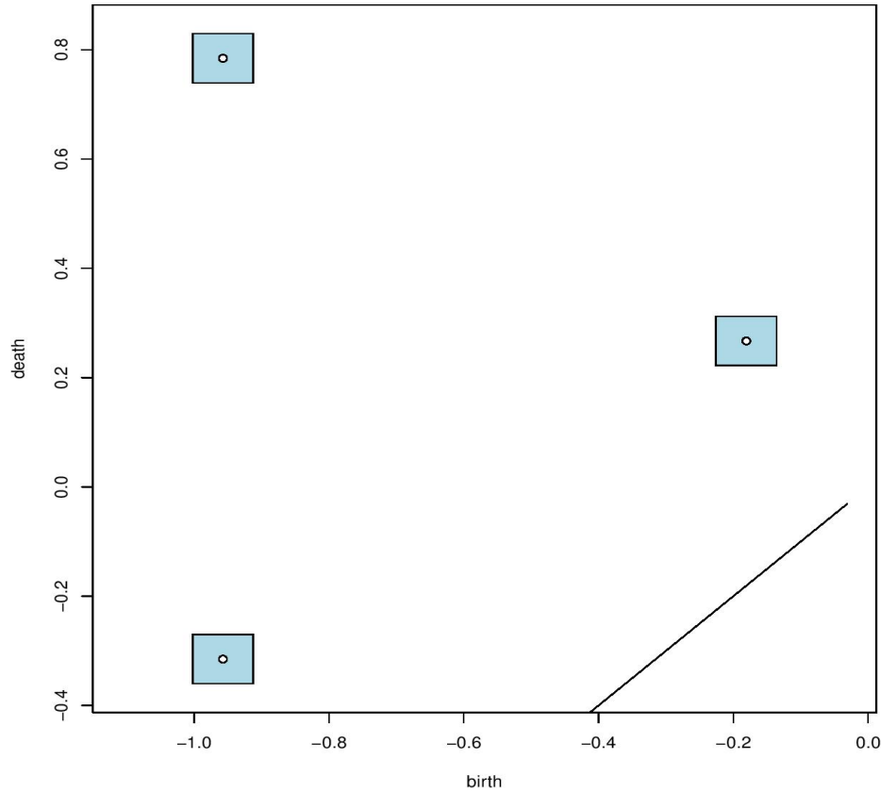
Or bootstrap (only empirical):

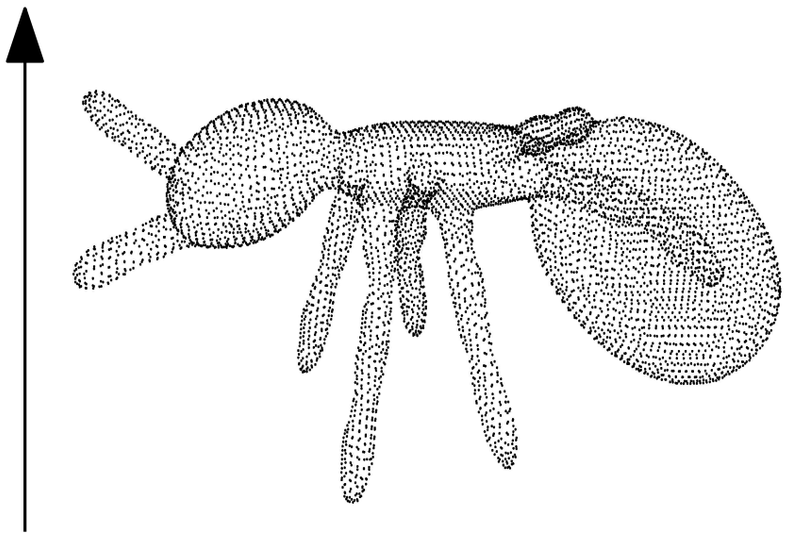
- draw $\widehat{X}_n^* = X_1^*, \cdots, X_n^*$ iid from $\mu_{\widehat{X}_n}$ (empirical measure on $\widehat{X}_n$)
- compute $\mathrm{d}^* = \mathrm{d}_B\left(\mathrm{M}_f(\widehat{X}_n^*), \mathrm{M}_f(\widehat{X}_n)\right)$
- repeat N times to get $\mathrm{d}_1^*, \cdots, \mathrm{d}_N^*$
- let q_α be the $(1-\alpha)$ quantile of $\frac{1}{N}\sum_{i=1}^N \mathbb{I}(\sqrt{n}\,\mathrm{d}_i^* \geq t)$
- take $c_n(\alpha) = \frac{q_\alpha}{\sqrt{n}}$

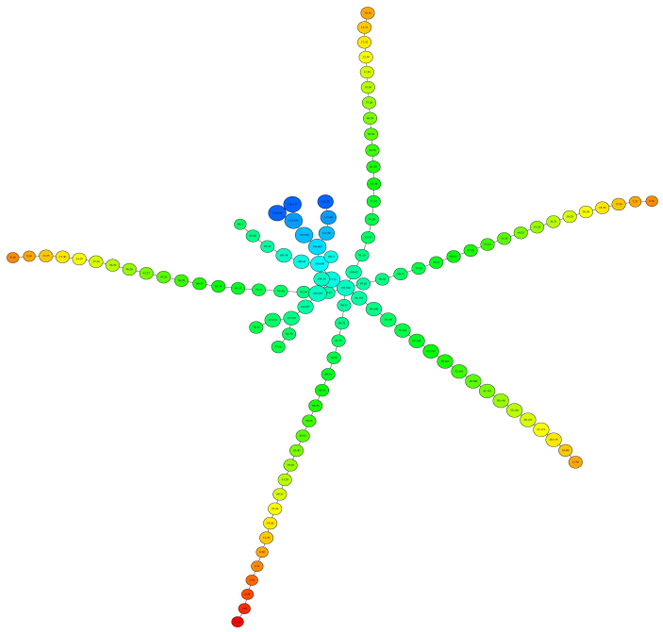
Experiments

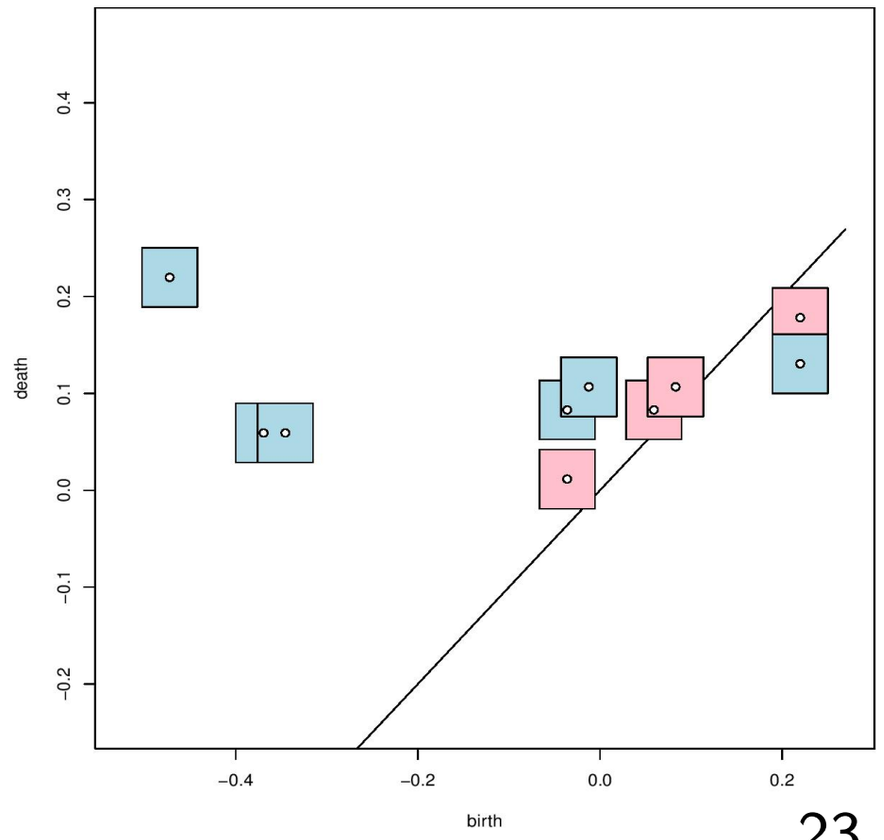




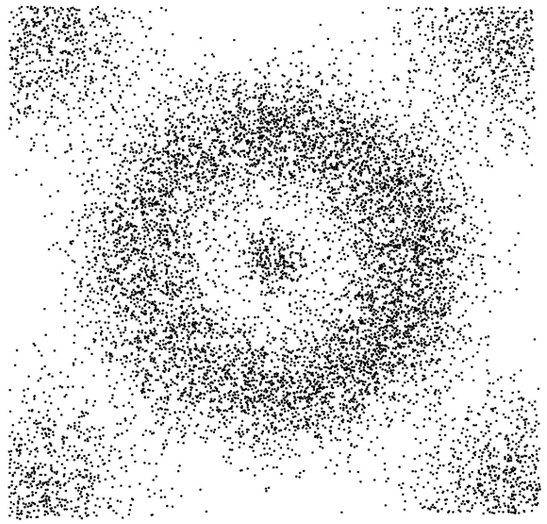


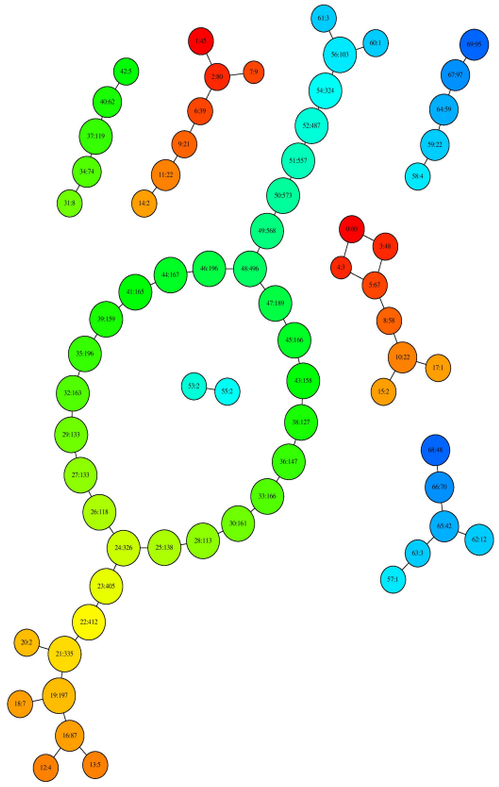


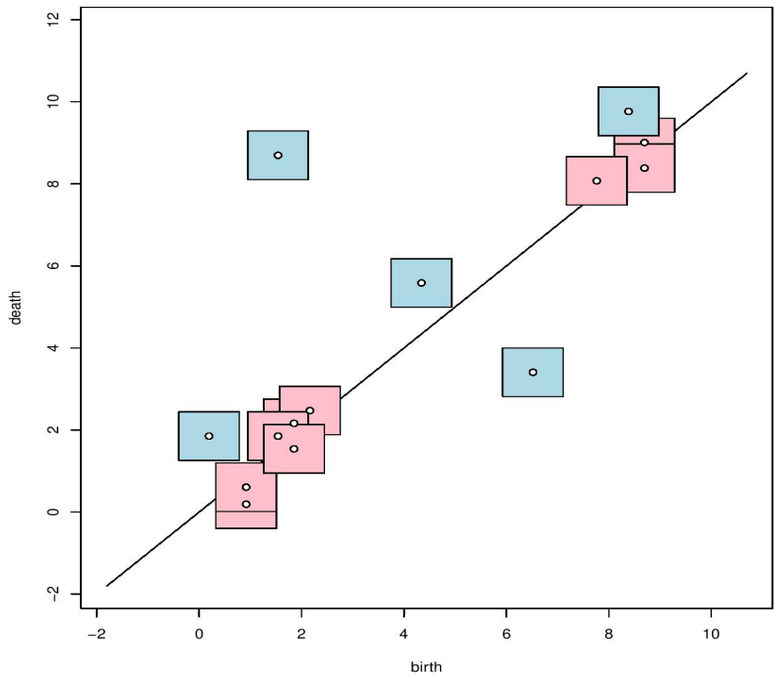


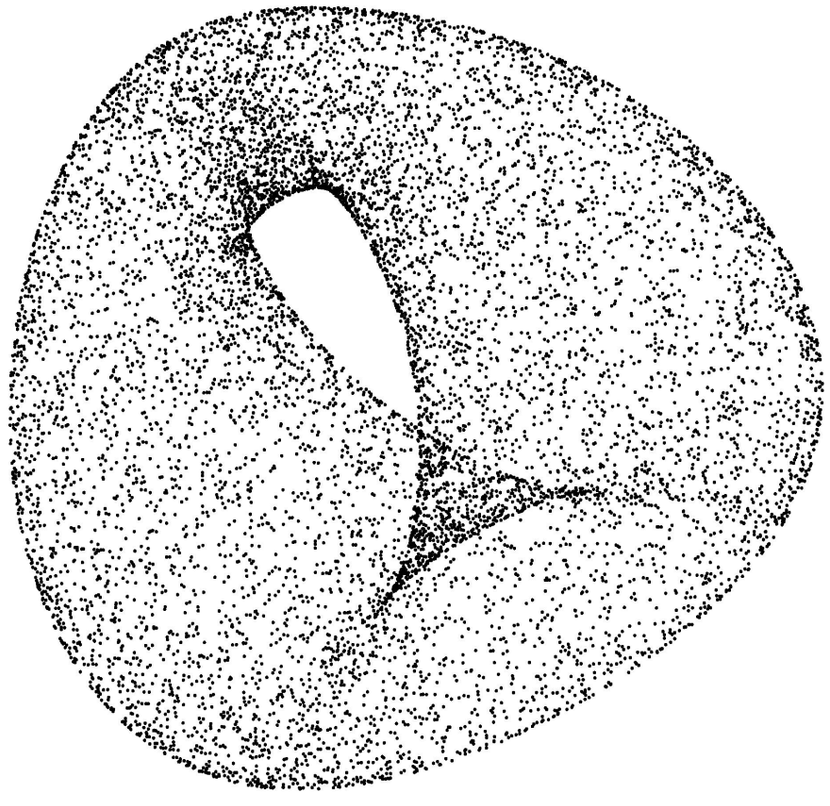


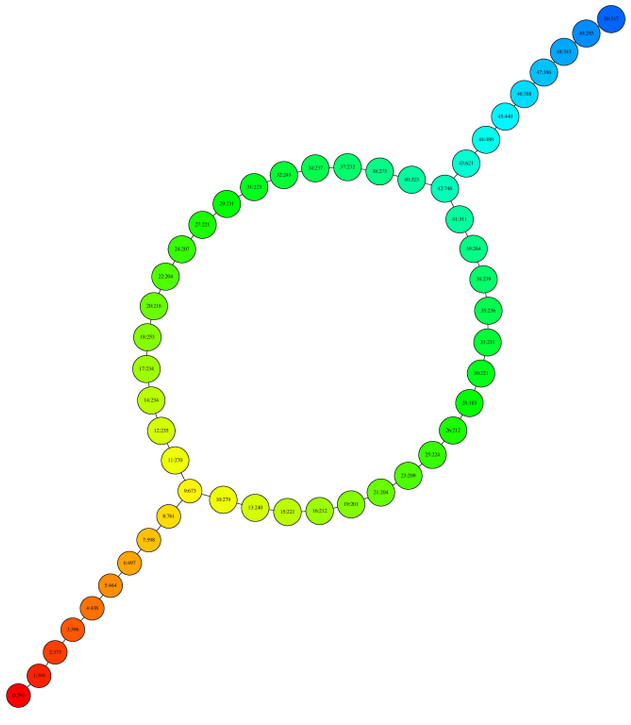
Experiments

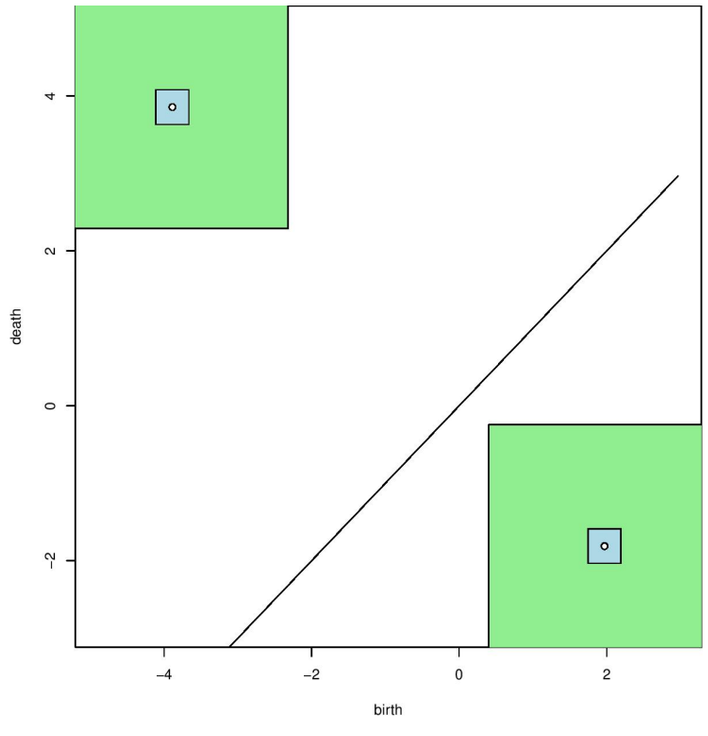




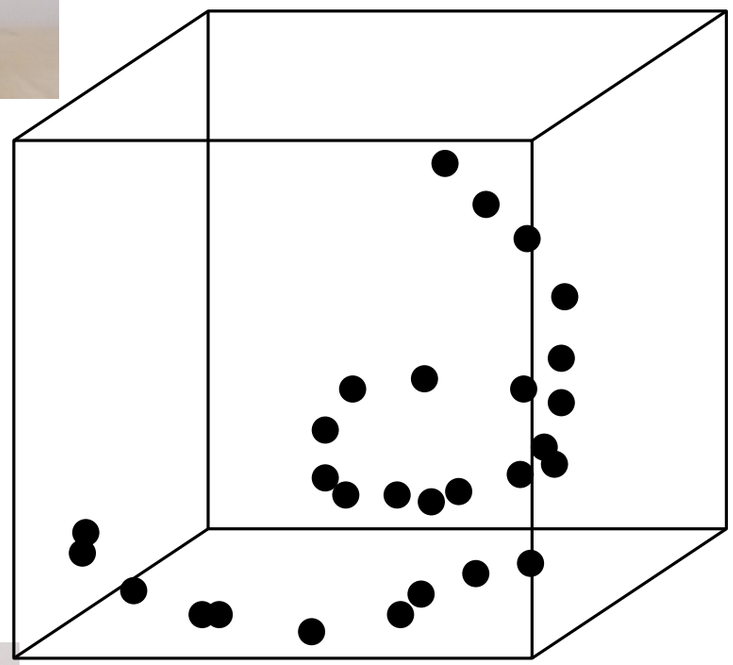


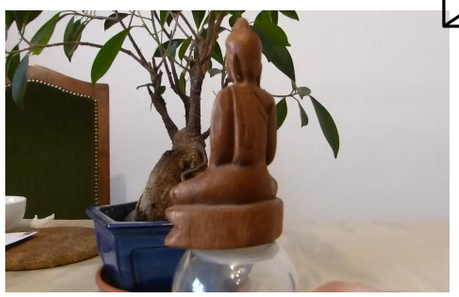




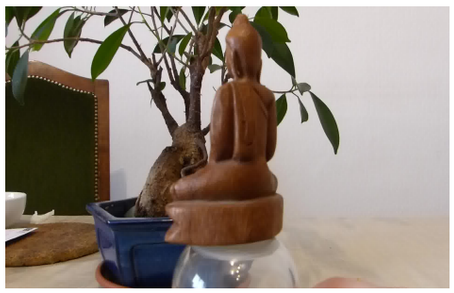


Experiments

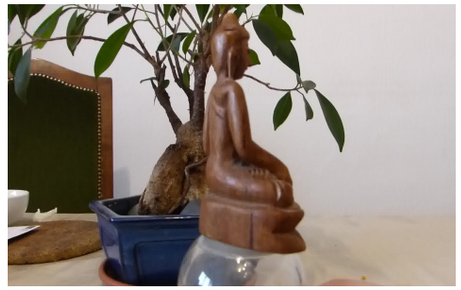


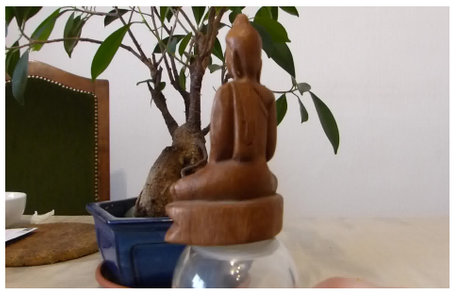


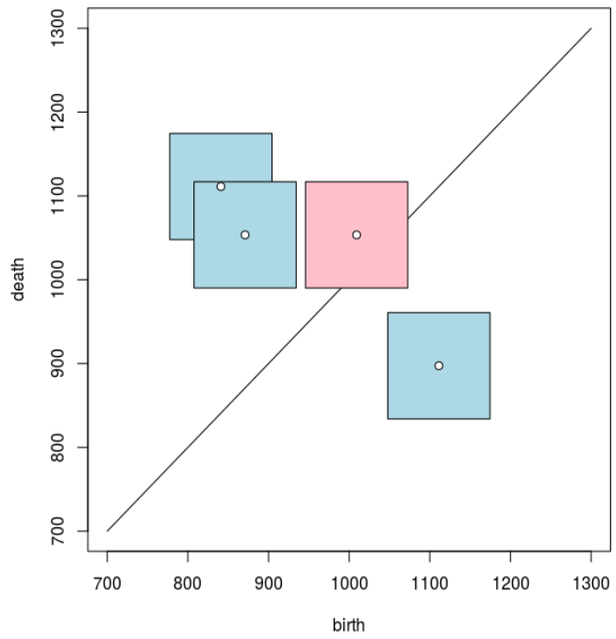
Experiments



Experiments







Learning

Learning is also possible *directly on Persistence Diagrams*

Kernel methods can compensate 'bad' properties of d_B and d_W^p

Learning

Learning is also possible *directly on Persistence Diagrams*

Kernel methods can compensate 'bad' properties of d_B and d_W^p

Finite-dimensional embedding: [C., Oudot, Ovsjanikov 2015]

Concatenate pairwise distances of Dg into single vector $\Phi(\mathrm{Dg})$

Thm: $\|\Phi(\mathrm{Dg}) - \Phi(\mathrm{Dg}')\|_\infty \leq 2\,\mathrm{d}_B(\mathrm{Dg}, \mathrm{Dg}')$

Learning

Learning is also possible *directly on Persistence Diagrams*

Kernel methods can compensate 'bad' properties of d_B and d_W^p

Finite-dimensional embedding: [C., Oudot, Ovsjanikov 2015]

Concatenate pairwise distances of Dg into single vector $\Phi(\mathrm{Dg})$

Thm: $\|\Phi(\mathrm{Dg}) - \Phi(\mathrm{Dg}')\|_\infty \leq 2\,\mathrm{d}_B(\mathrm{Dg}, \mathrm{Dg}')$

Gaussian Kernel: [C., Cuturi, Oudot 2017]

Modify d_W^1 into SW and use $\exp\left(-\frac{\mathrm{SW}(\cdot,\cdot)}{2\sigma^2}\right)$

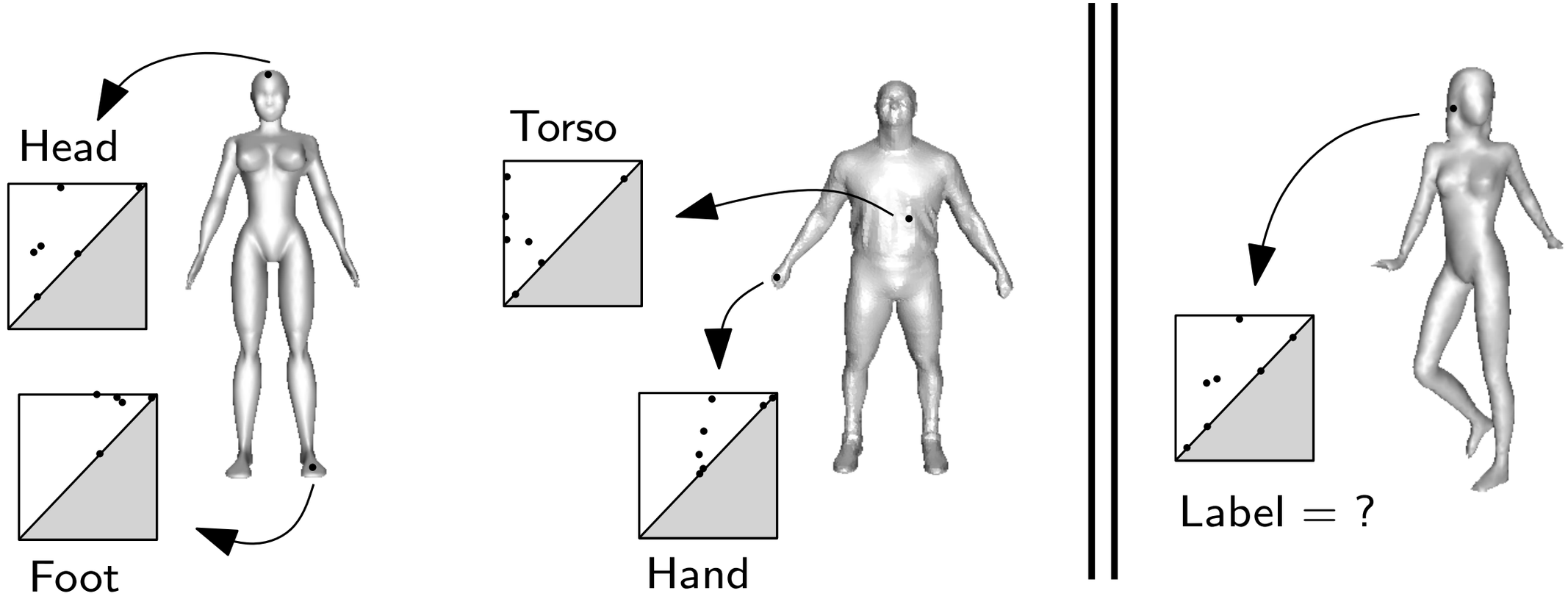
Thm: $C(N)\,\mathrm{d}_W^1(\mathrm{Dg}, \mathrm{Dg}') \leq \mathrm{SW}(\mathrm{Dg}, \mathrm{Dg}') \leq 2\sqrt{2}\,\mathrm{d}_W^1(\mathrm{Dg}, \mathrm{Dg}')$

Application to supervised shape segmentation

Goal: segment 3d shapes based on examples

Approach:

- train a (multiclass) classifier on PDs extracted from the training shapes
- apply classifier to PDs extracted from query shape



Application to supervised shape segmentation

Goal: segment 3d shapes based on examples

Approach:

- train a (multiclass) classifier on PDs extracted from the training shapes
- apply classifier to PDs extracted from query shape

Accuracies (%):

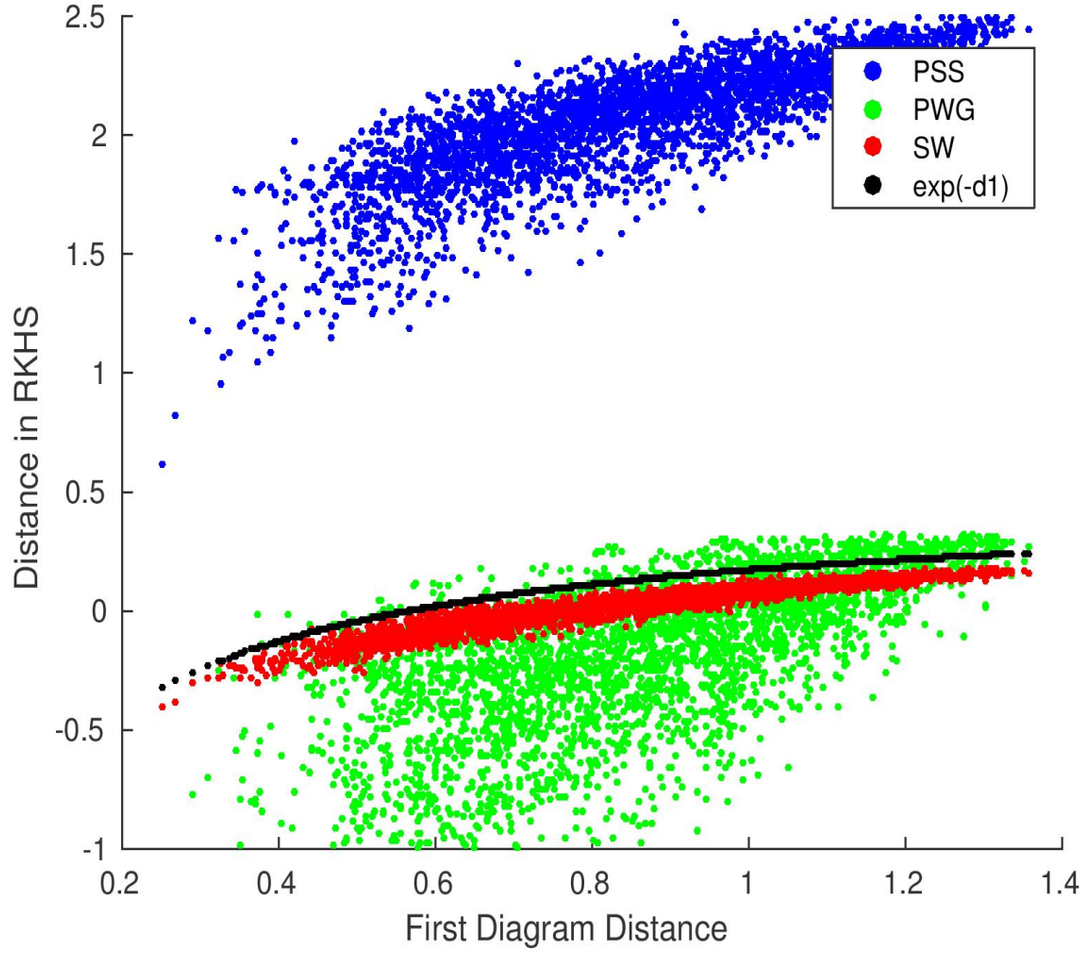
	TDA	geometry	TDA + geometry
Human	74.0	78.7	**88.7**
Airplane	72.6	81.3	**90.7**
Ant	92.3	90.3	**98.5**
FourLeg	73.0	74.4	**84.2**
Octopus	85.2	94.5	**96.6**
Bird	72.0	75.2	**86.5**
Fish	79.6	79.1	**92.3**

Application to supervised shape segmentation

Goal: segment 3d shapes based on examples

Approach:

- train a (multiclass) classifier on PDs extracted from the training shapes
- apply classifier to PDs extracted from query shape



Conclusion

Structure and Stability of Mapper

Parameter Selection for Mapper

Kernel Methods for Persistence Diagrams

Extensions:

Multivariate function $f : X \to \mathbb{R}^n$

Space of Reeb graphs (curvature, barycenters, interpolation...)

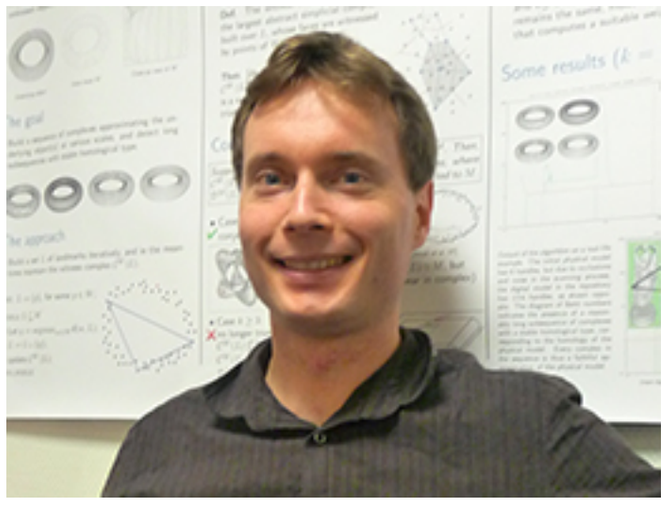
Other types of statistics for Persistence Diagrams/Mappers

Many thanks to:

Maks Ovsjanikov

Bertrand Michel

Marco Cuturi



Steve Oudot

गुढी GUDHI

DAAD

ÉCOLE DOCTORALE

Sciences et technologies
de l'information
et de la communication (STIC)