Abel Symposium
Geiranger, June 2018

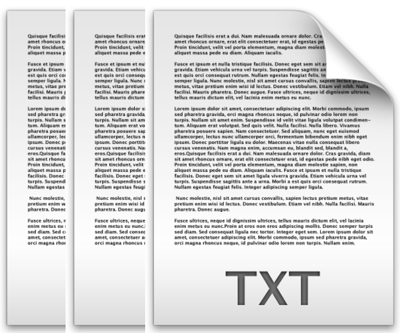
On Inverse Problems in TDA

Steve Oudot

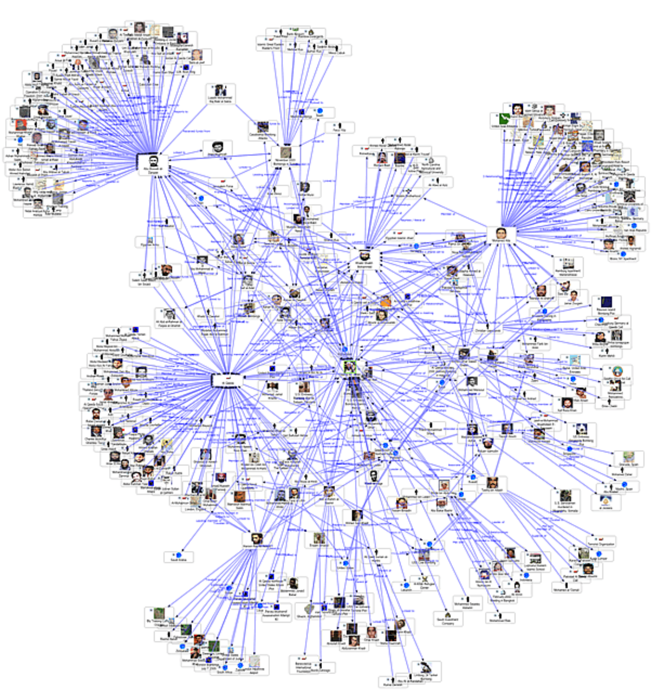
Inria

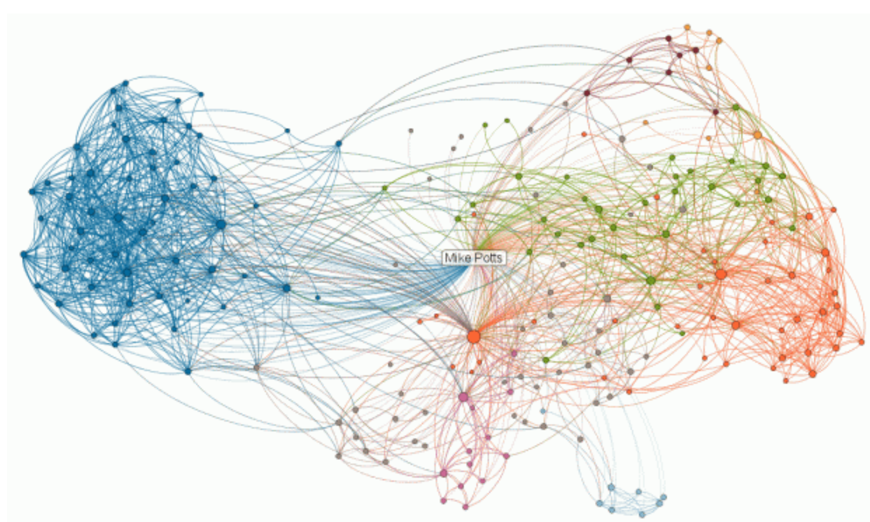
— joint work with E. Solomon (Brown Math.) — arXiv: 1712.03630

The preimage problem in the data Sciences



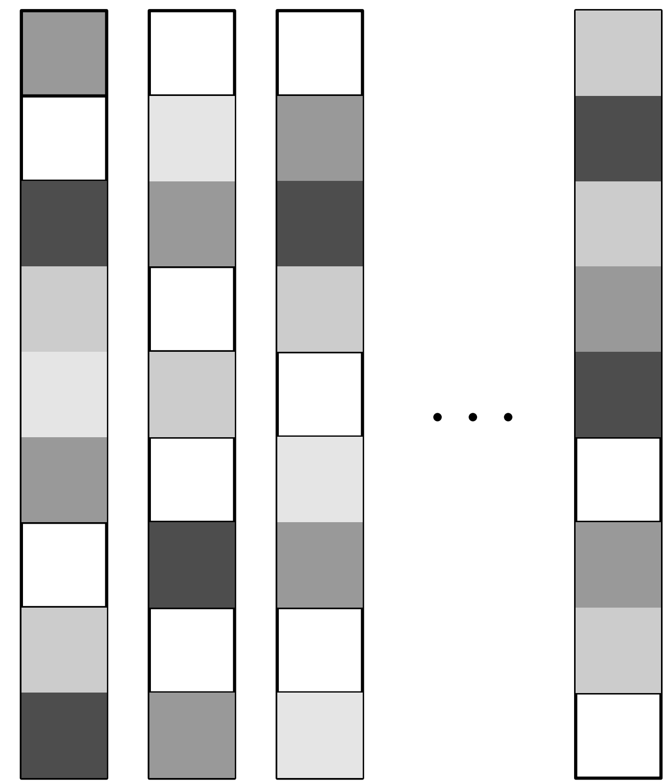
Data





(feature design or learning)

Features $\in \mathbb{R}^n$



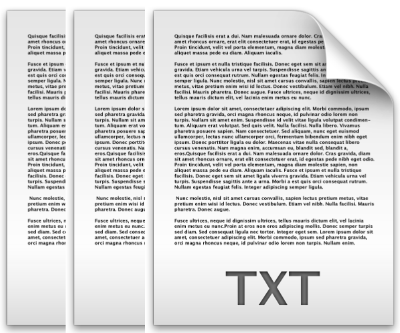
bag of words, word2vec

shape contexts, heat kernels

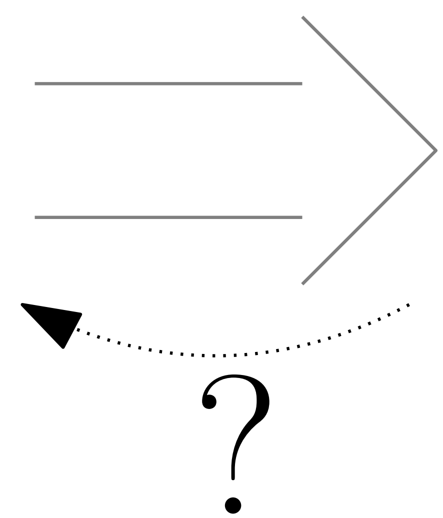
node2vec, Laplacian fact., rand. walks

dim. reduction, auto-encoders, etc.

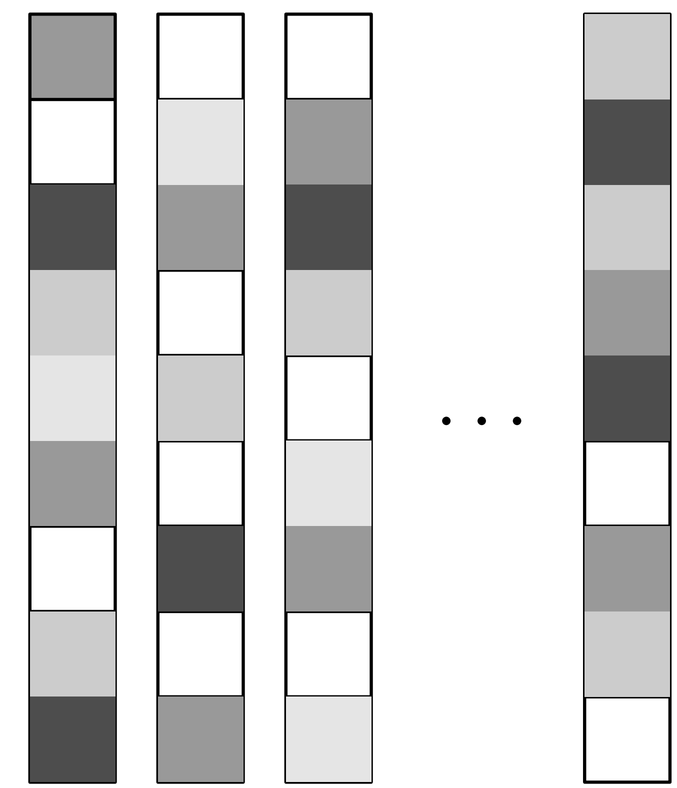
The preimage problem in the data Sciences

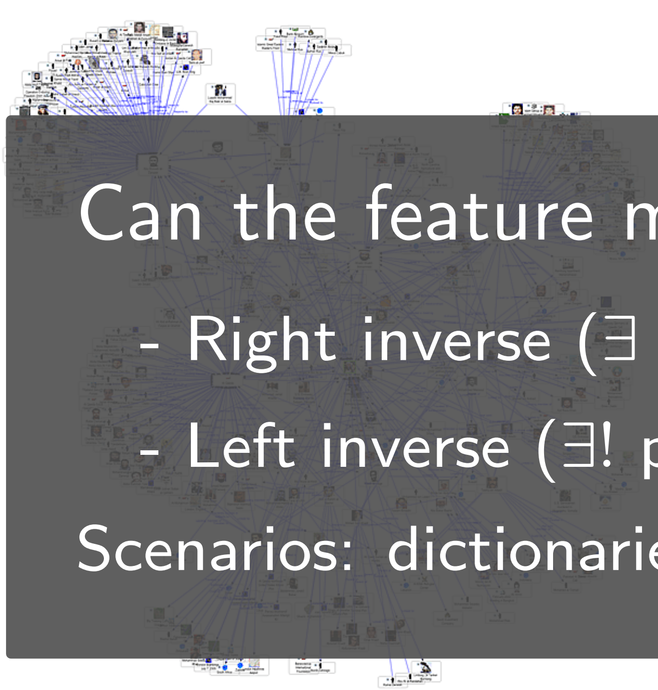


Data



Features $\in \mathbb{R}^n$





Can the feature map be inverted?

- Right inverse ($\exists$ preimage): interpretable AI
- Left inverse ($\exists!$ preimage): reliable interpretation

Scenarios: dictionaries, deep layers, stats, etc.

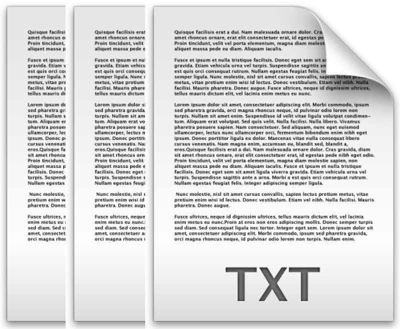
bag of words, word2vec

shape contexts, heat kernels

node2vec, Laplacian fact., rand. walks

dim. reduction, auto-encoders, etc.

The preimage problem in the data Sciences

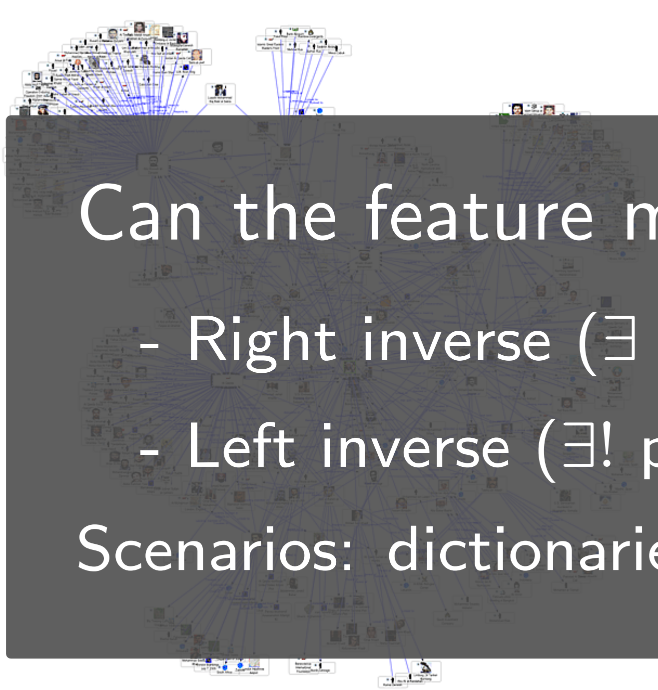


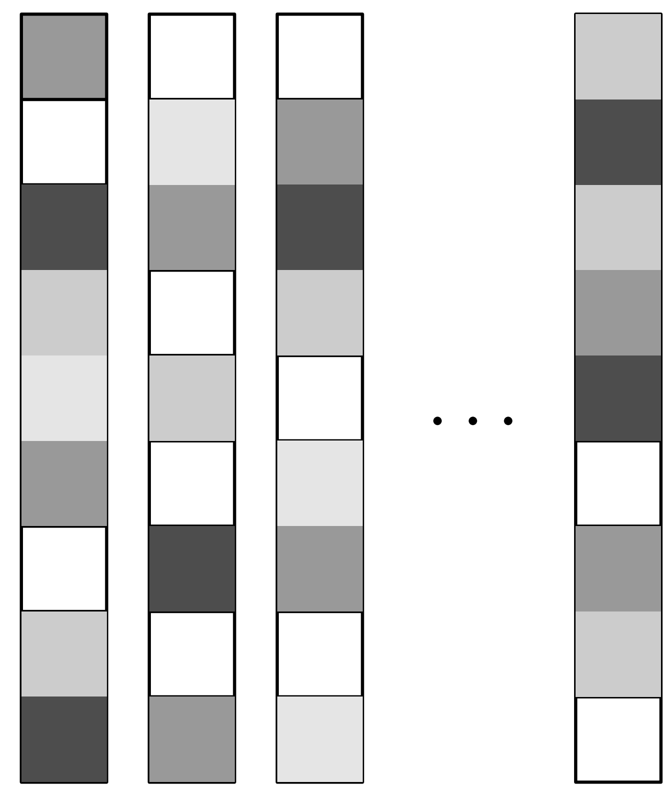
Data

Features $\in \mathbb{R}^n$

(feature design or learning)

?



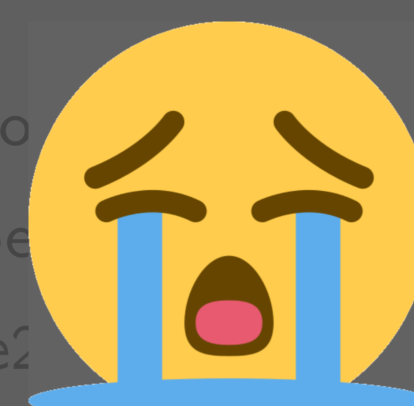


. . .

Can the feature map be inverted?

- Right inverse (∃ preimage): interpretable AI
- Left inverse (∃! preimage): reliable interpretation

Scenarios: dictionaries, deep layers, stats, etc.



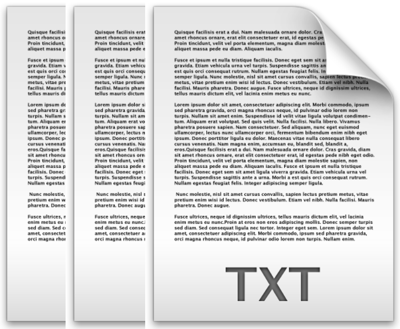
bag o … 2vec

shape … t kernels

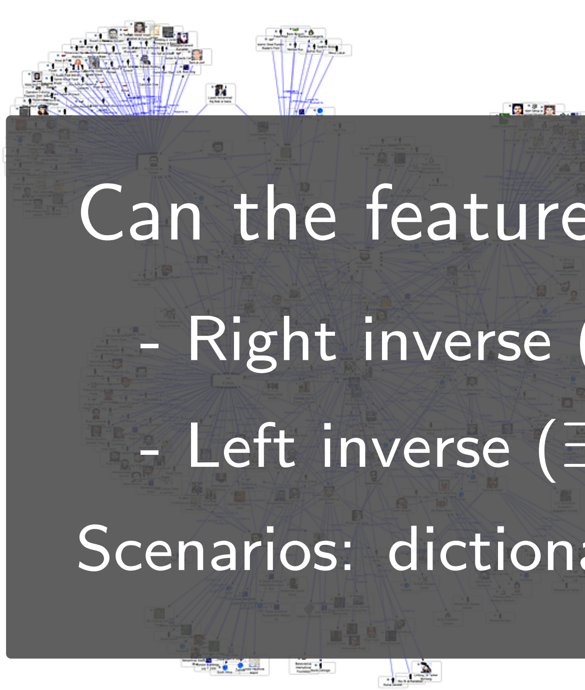
node2 … fact., rand. walks

dim. reduction, auto-encoders, etc.

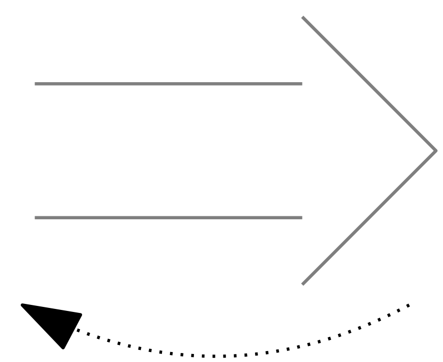
The preimage problem in the data Sciences



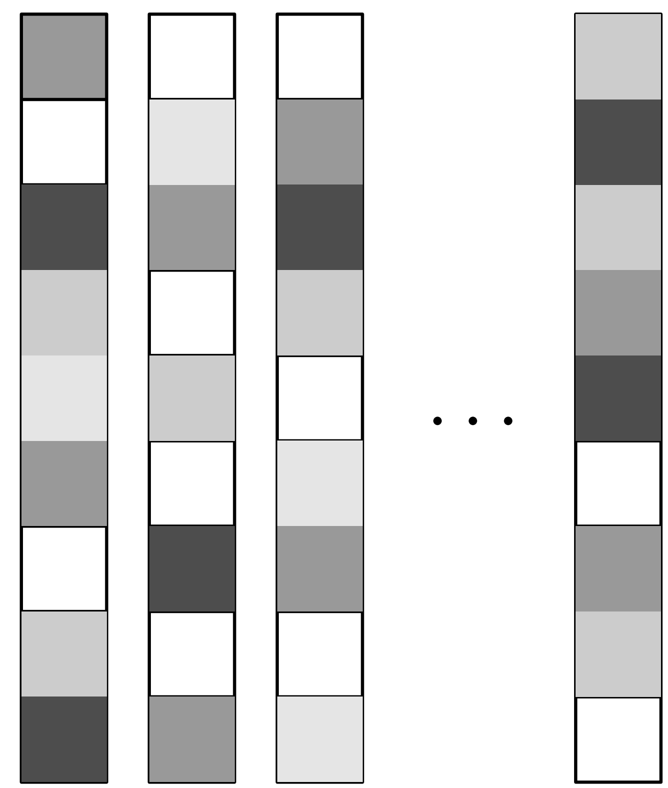
Data



(feature design or learning)



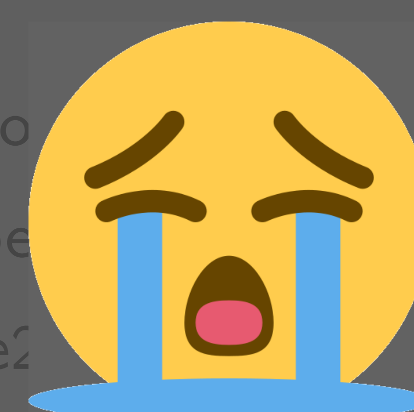
Features $\in \mathbb{R}^n$

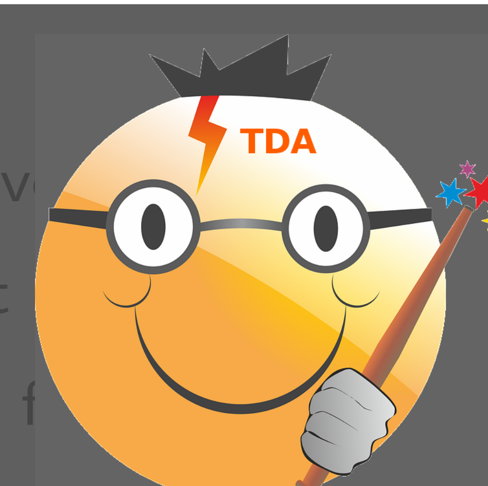


Can the feature map be inverted?

- Right inverse ($\exists$ preimage): interpretable AI
- Left inverse ($\exists!$ preimage): reliable interpretation

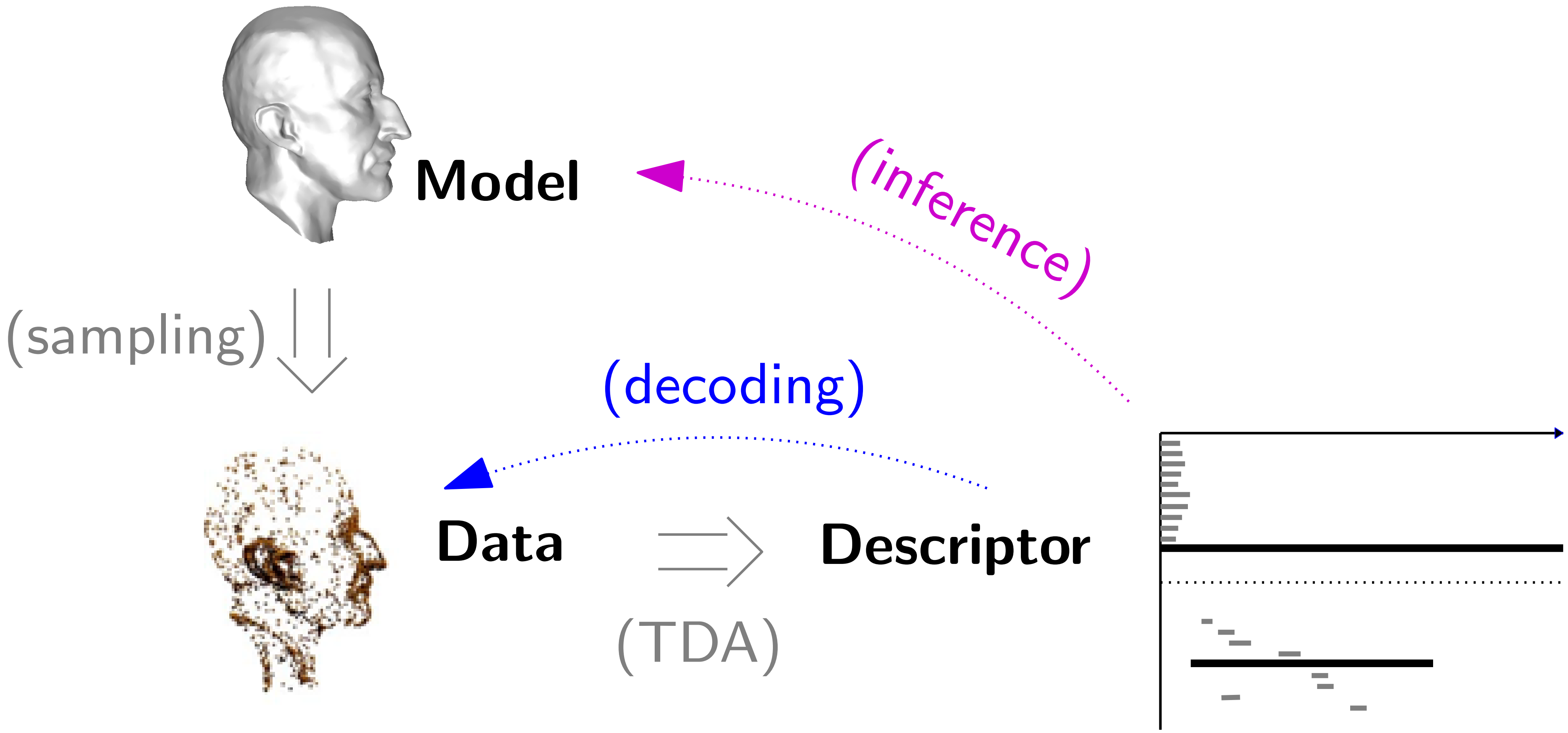
Scenarios: dictionaries, deep layers, stats, etc.





dim. reduction, auto-encoders, etc.

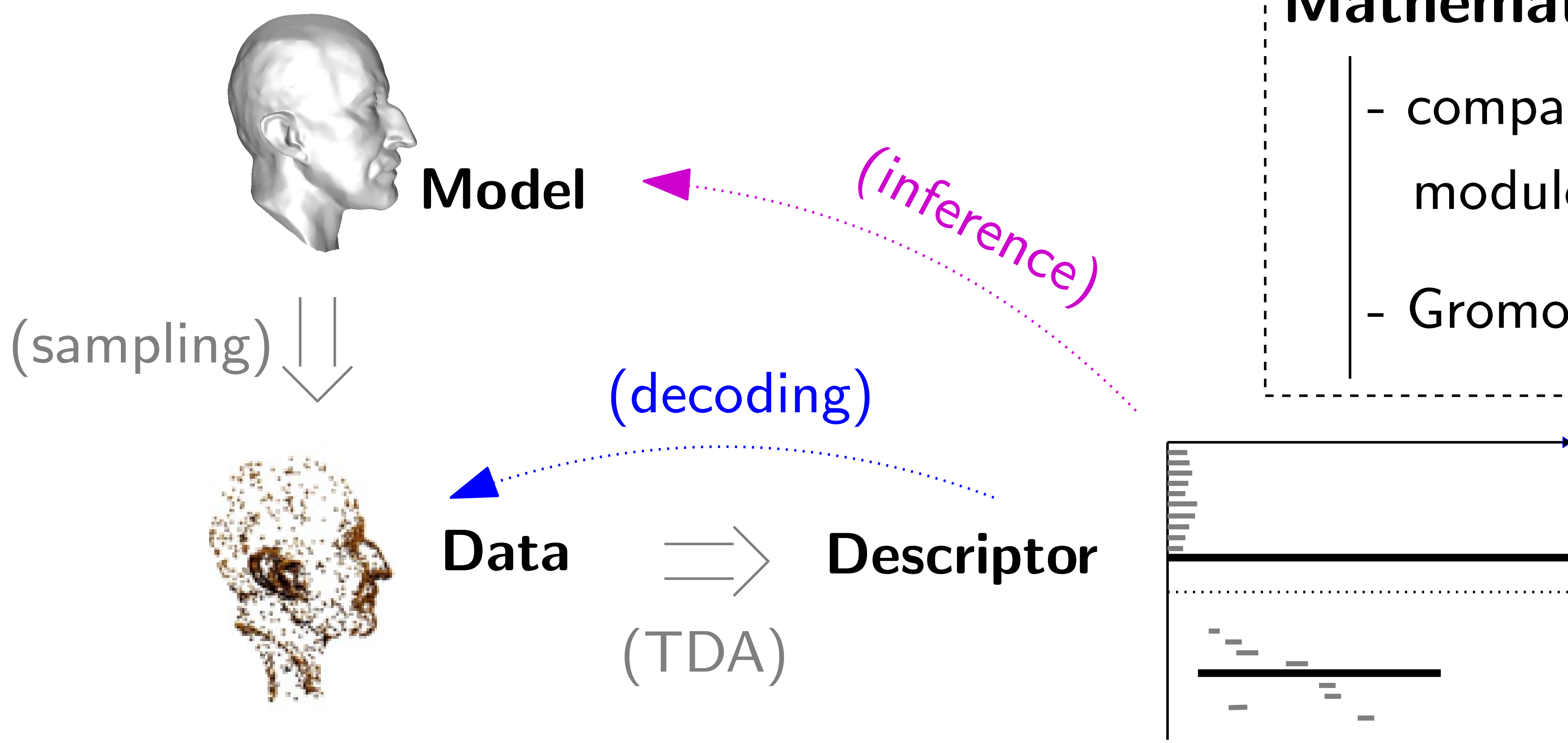
TDA and the preimage problem

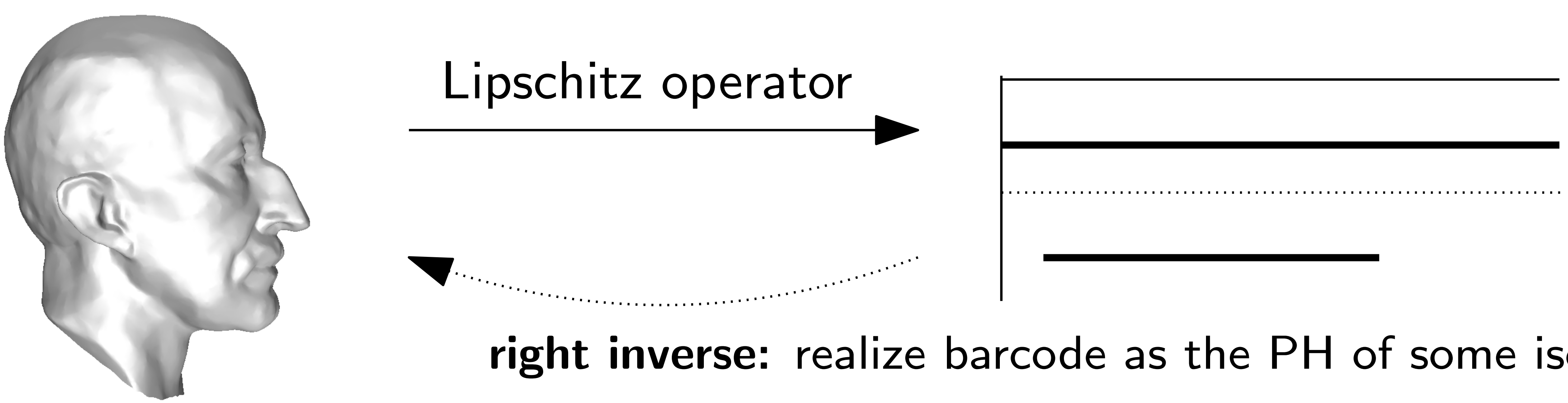


TDA and the preimage problem

Mathematical abstraction:

- compact metric spaces modulo isometries
- Gromov-Hausdorff distance



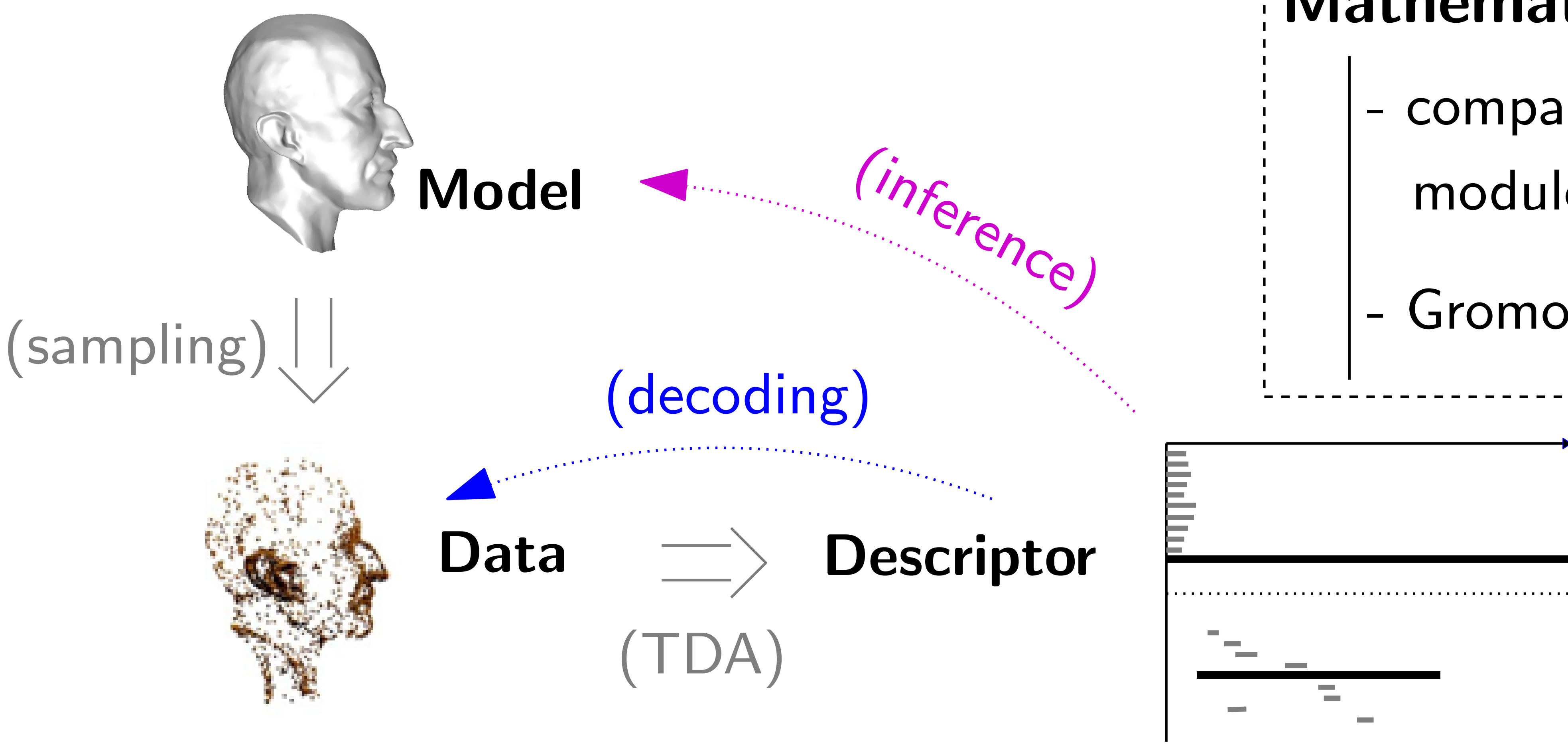


compact metric space

right inverse: realize barcode as the PH of some isom. class

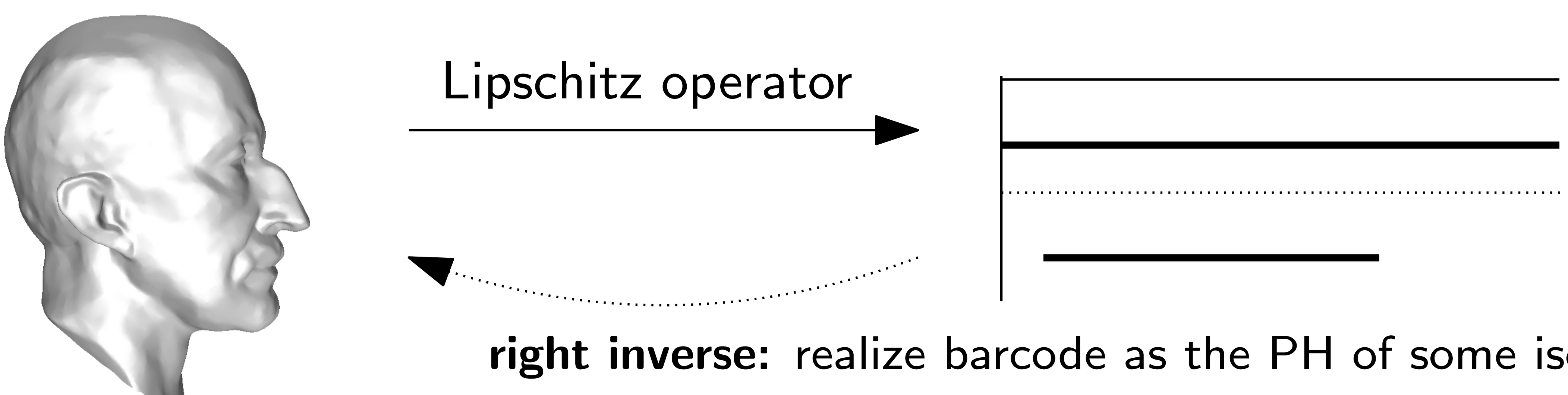
left inverse: characterize isom. class uniquely

TDA and the preimage problem



Mathematical abstraction:

- compact metric spaces modulo isometries
- Gromov-Hausdorff distance



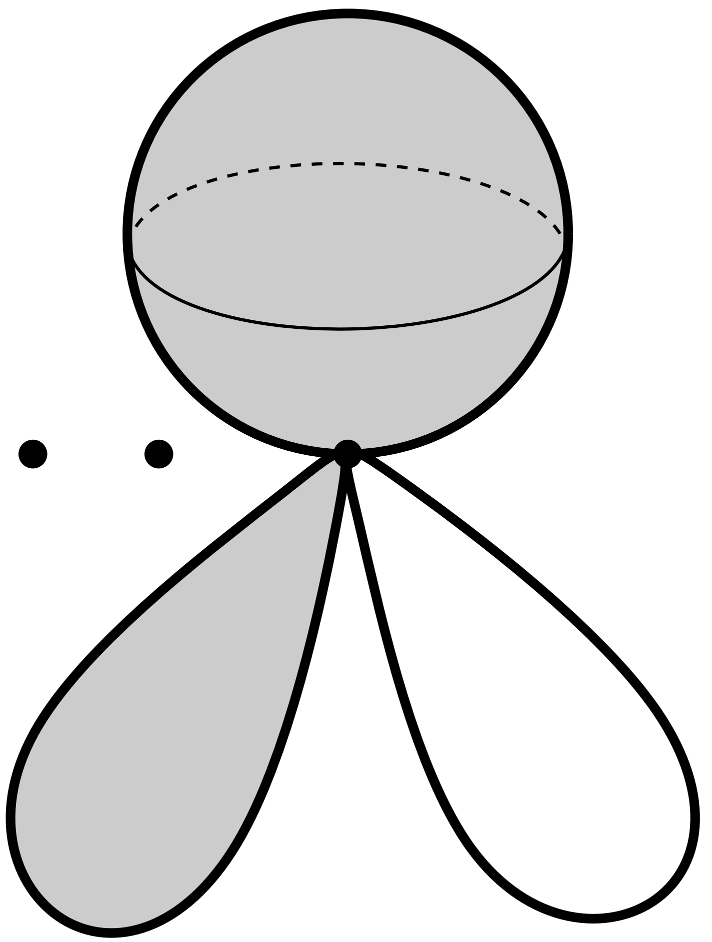
compact metric space

right inverse: realize barcode as the PH of some isom. class

left inverse: characterize isom. class uniquely

Right inverses for TDA

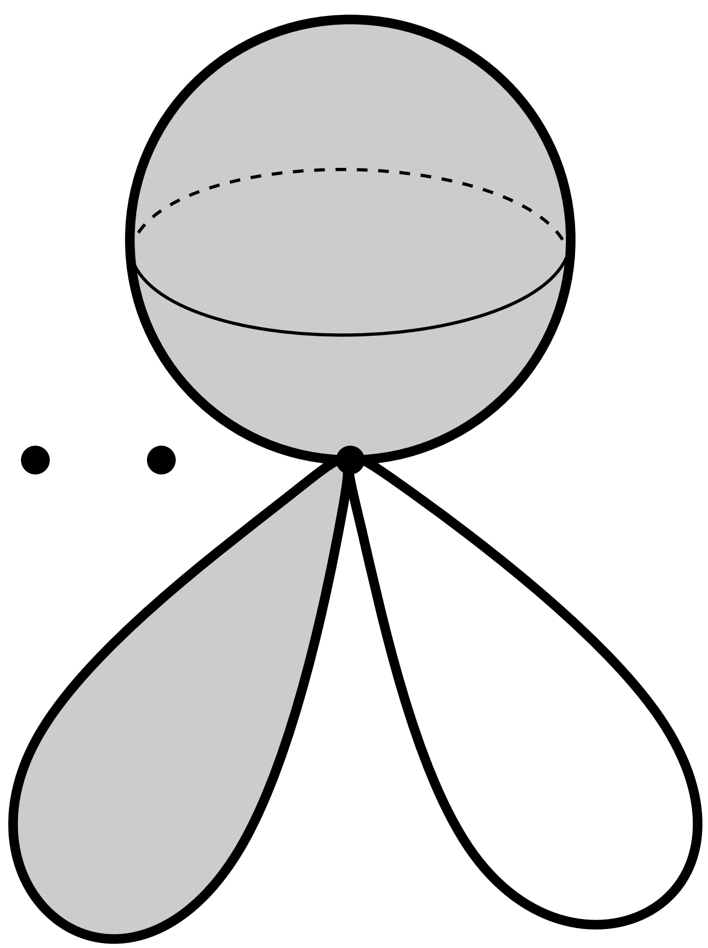
Fact: [Folklore] Any (graded) persistence module $\mathbb{R} \to \mathrm{vect}_{\boldsymbol{k}}$ can be realized as the (graded) $\mathrm{P\tilde{H}}$ of a piecewise-constant function on a bouquet of spheres.

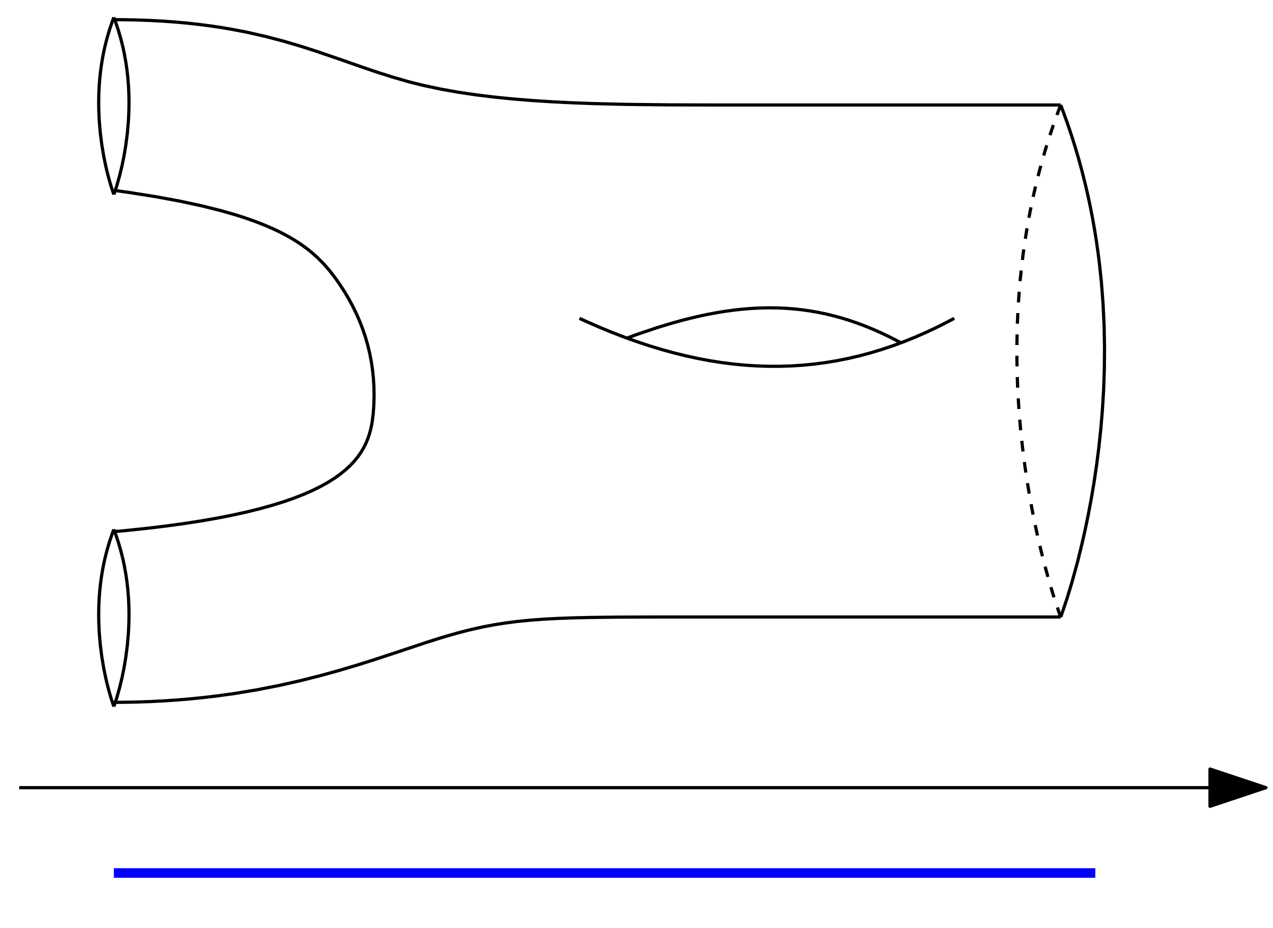


Right inverses for TDA

Fact: [Folklore] Any (graded) persistence module $\mathbb{R} \to \mathrm{vect}_{\Bbbk}$ can be realized as the (graded) P$\tilde{\mathrm{H}}$ of a piecewise-constant function on a bouquet of spheres.

Thm: [Curry, Reiss] [Botnan, Fluhr]
Any (graded) barcode can be realized as the level-set P$\tilde{\mathrm{H}}$ of some stratified map on some stratified space.





Right inverses (local) for TDA

point cloud — Čech / Rips filtration — barcode

$$u \in \mathbb{R}^{nd} \longmapsto v \in \mathbb{R}^{2^n - 1}$$

Thm: [Gameiro, Hiraoka, Obayashi]

(i) *Generic* point cloud $\Rightarrow \exists \Omega \ni u$ in $\mathbb{R}^{nd}$ over which the correspondence $u \mapsto v$ can be extended to a map $f : \Omega \to \mathbb{R}^{2^n - 1}$ computing persistence barcodes.

(ii) For Ω small enough, f is of class C^∞.

Observation: pairing given by order of distances is constant in small enough O.

Right inverses (local) for TDA

point cloud   Čech / Rips filtration   barcode

$$u \in \mathbb{R}^{nd} \longmapsto v \in \mathbb{R}^{2^n-1}$$

Thm: [Gameiro, Hiraoka, Obayashi]

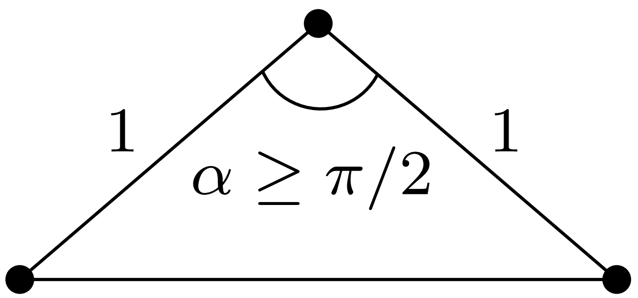
(i) *Generic* point cloud $\Rightarrow \exists \Omega \ni u$ in $\mathbb{R}^{nd}$ over which the correspondence $u \mapsto v$ can be extended to a map $f : \Omega \to \mathbb{R}^{2^n-1}$ computing persistence barcodes.

(ii) For Ω small enough, f is of class C^∞.

$\to$ adapt Newton-Raphson continuation method to build right inverse of f in $f(\Omega)$
(Jacobian matrix of f can be singular $\rightsquigarrow$ use pseudo-inverse)

Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations



$$\operatorname{dgm} \mathcal{C}(P, \ell_2) = \{(0, +\infty)\} \sqcup \{(0, \tfrac{1}{2})\} \sqcup \{(0, \tfrac{1}{2})\}$$

$$\operatorname{dgm} \mathcal{R}(P, \ell_2) = \{(0, +\infty)\} \sqcup \{(0, 1)\} \sqcup \{(0, 1)\}$$

$\Rightarrow$ diagrams for different values of α are indistinguishable

Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations

Prop: [Folklore]

For any *metric tree* (X, d_X):

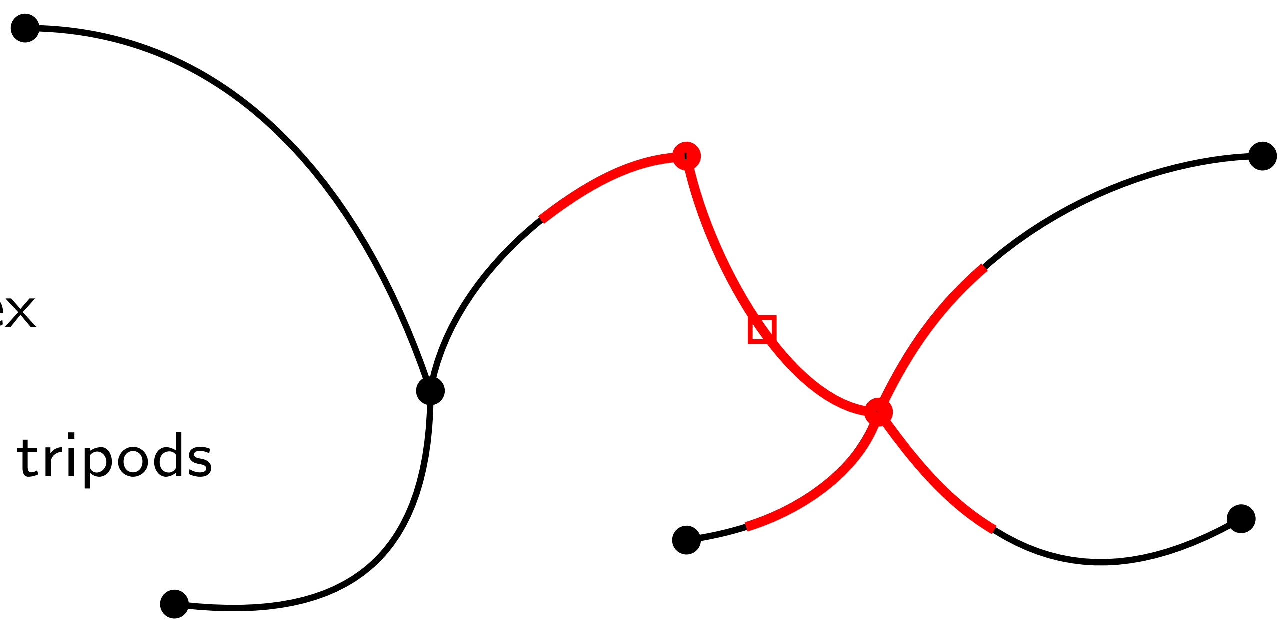
$$\mathrm{dgm}\,\mathcal{R}(X, \mathrm{d}_X) = \mathrm{dgm}\,\mathcal{C}(X, \mathrm{d}_X) = \{(0, +\infty)\}$$

$\Rightarrow$ no information on the metric

X is 0-hyperbolic

$\Rightarrow$ metric balls are convex

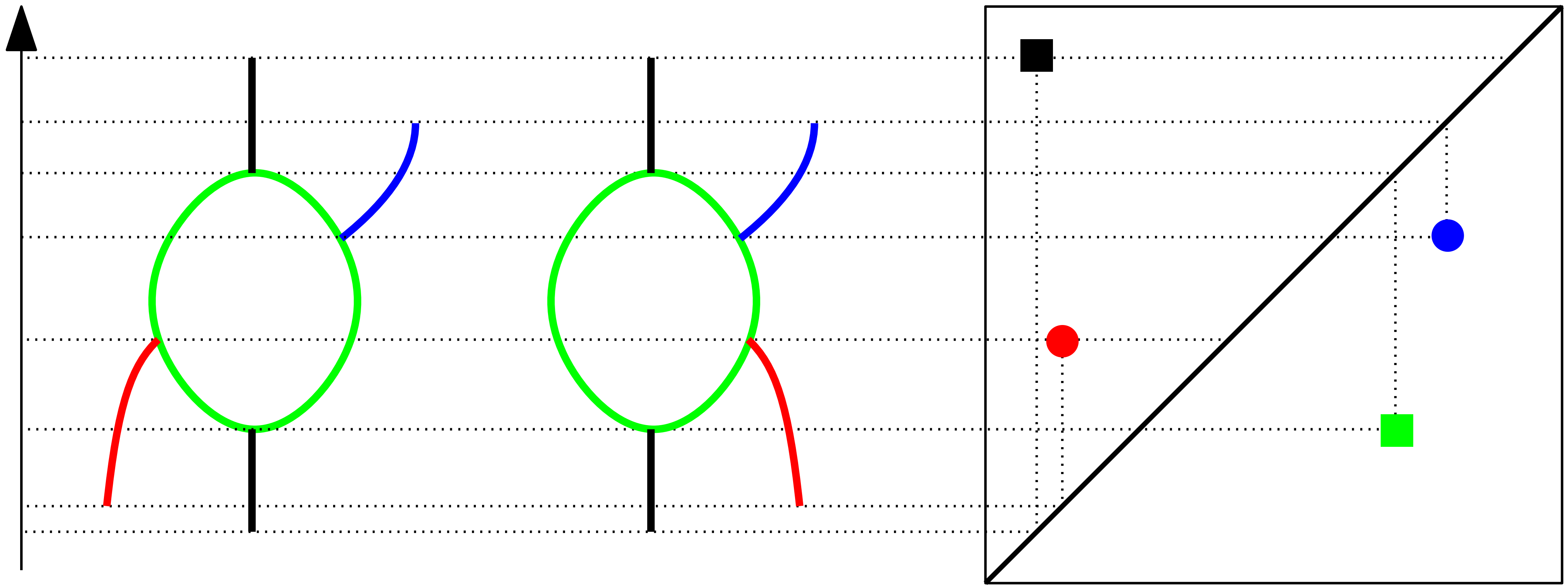
$\Rightarrow$ geodesic triangles are tripods



Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations

- Reeb graphs



⇒ Reeb graphs are indistinguishable from their diagrams

Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations
- Reeb graphs
- Real-valued functions

Prop: [Folklore]

Given $f : X \to \mathbb{R}$ and $h : Y \to X$ homeomorphism,

$$\operatorname{dgm} f \circ h = \operatorname{dgm} f$$

Too large a group of transformations...

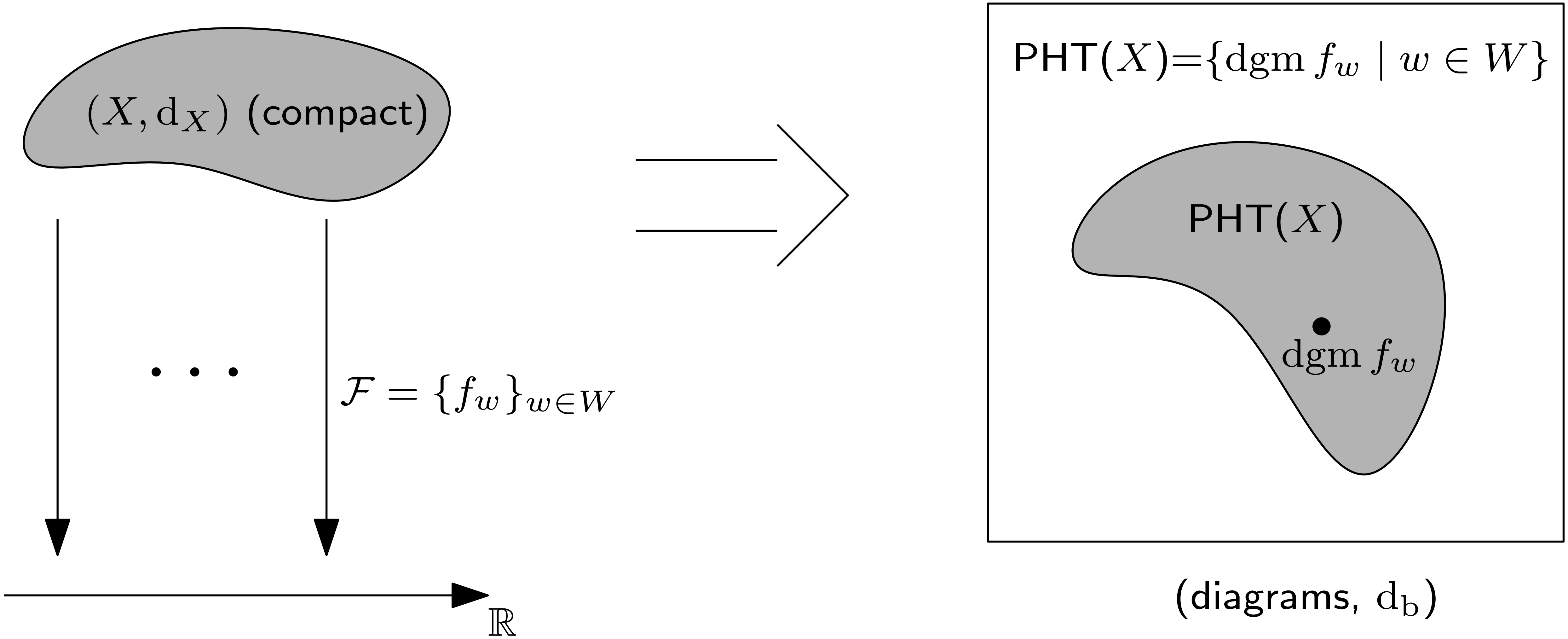
Left inverses?

- Unions of (open) balls — Čech/Rips/Delaunay filtrations
- Reeb graphs
- Real-valued functions

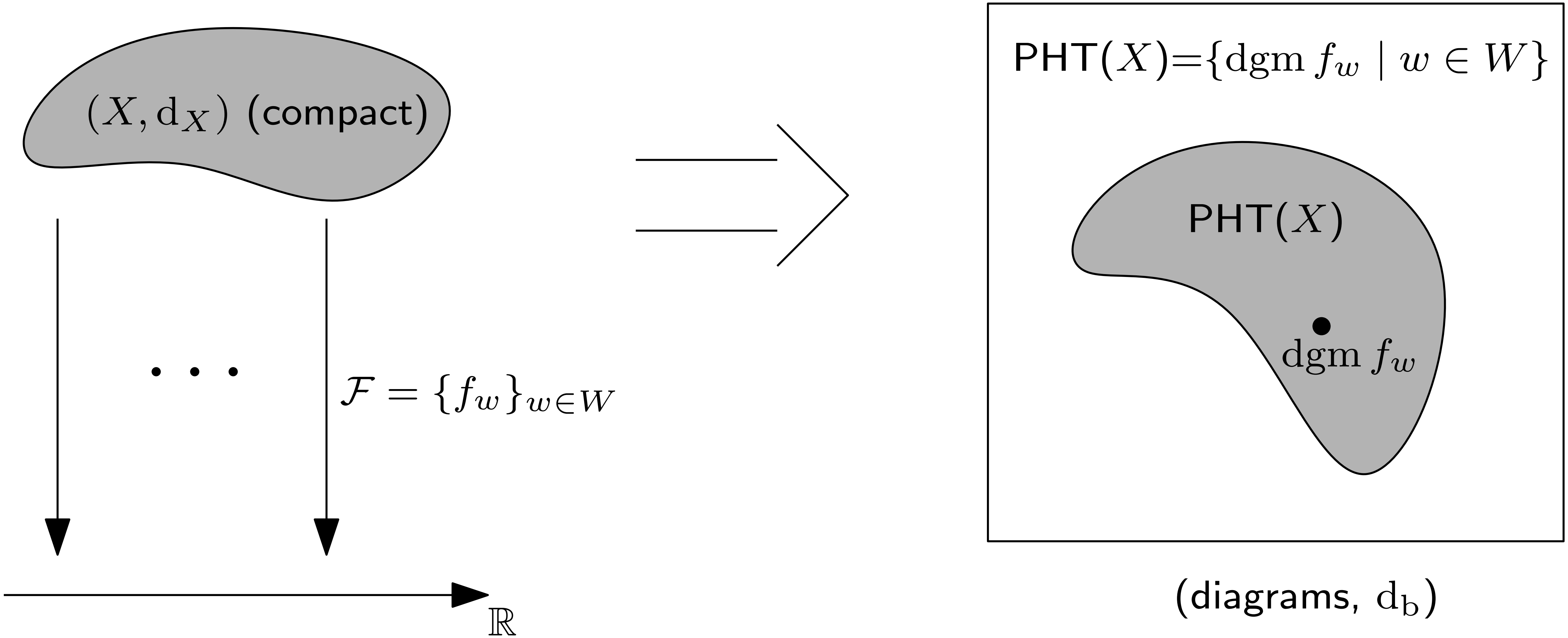
possible solutions:

- richer topological invariants (e.g. persistent homotopy)
- use multiple filter functions (**aggregation** vs multipersistence)

Persistent Homology Transform (PHT)



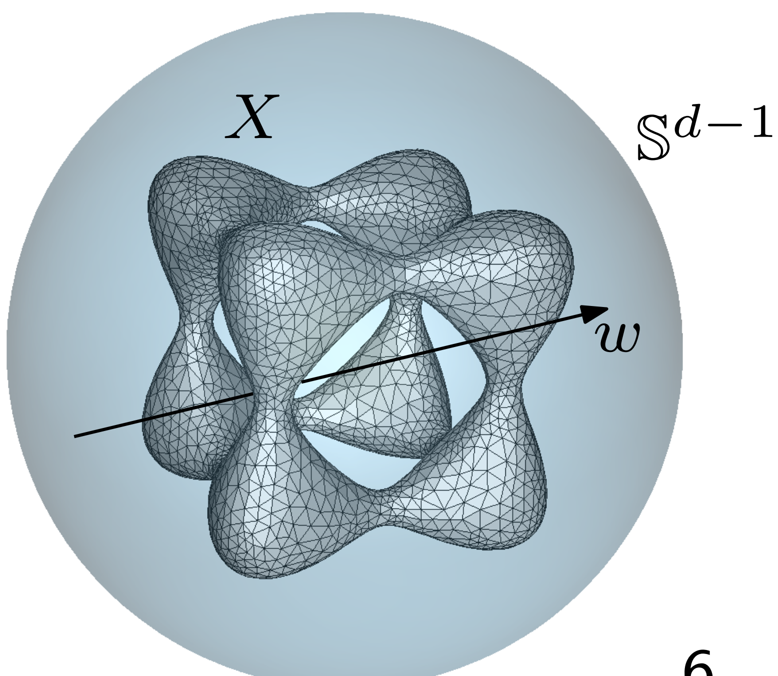
Persistent Homology Transform (PHT)



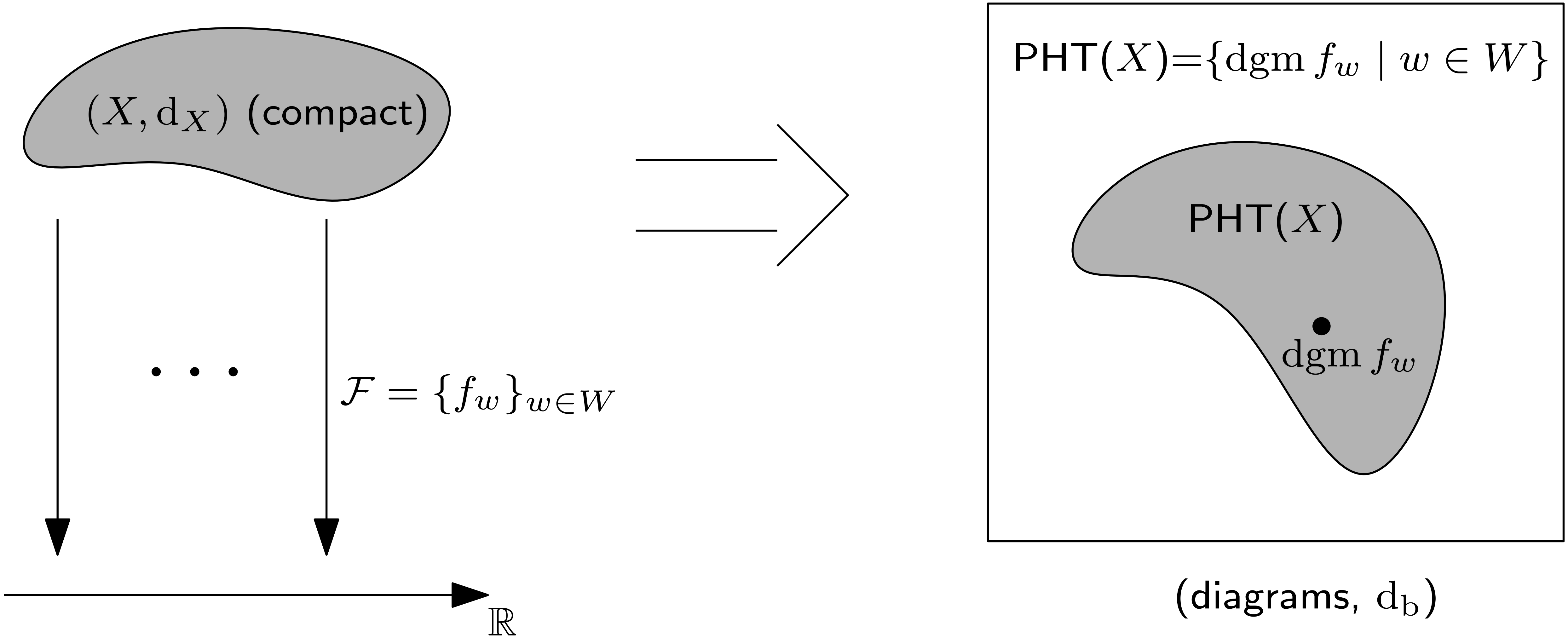
Thm: [Boyer, Curry, Mukherjee, Turner 2014, 2018]
[Ghrist, Levanger, Mai 2018]

Let $\mathcal{F} = \{\langle \cdot, w \rangle\}_{w \in \mathbb{S}^{d-1}}$, where d is fixed. Then, PHT is injective on the class of semialgebraic sets in $\mathbb{R}^d$.

Still true for a fixed finite set of directions (of size exponential in d). [Curry, Mukherjee, Turner]



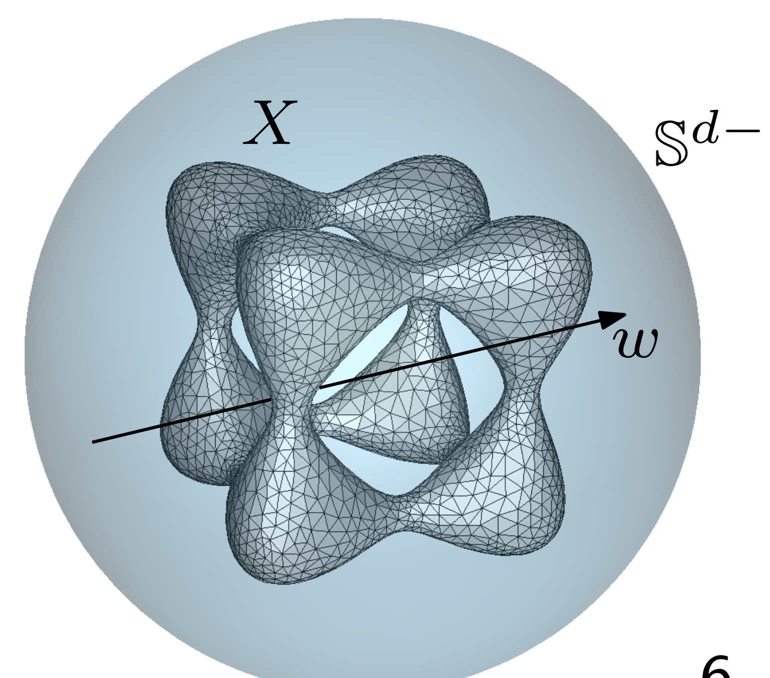
Persistent Homology Transform (PHT)



Thm: [Boyer, Curry, Mukherjee, Turner 2014, 2018]
[Ghrist, Levanger, Mai 2018]

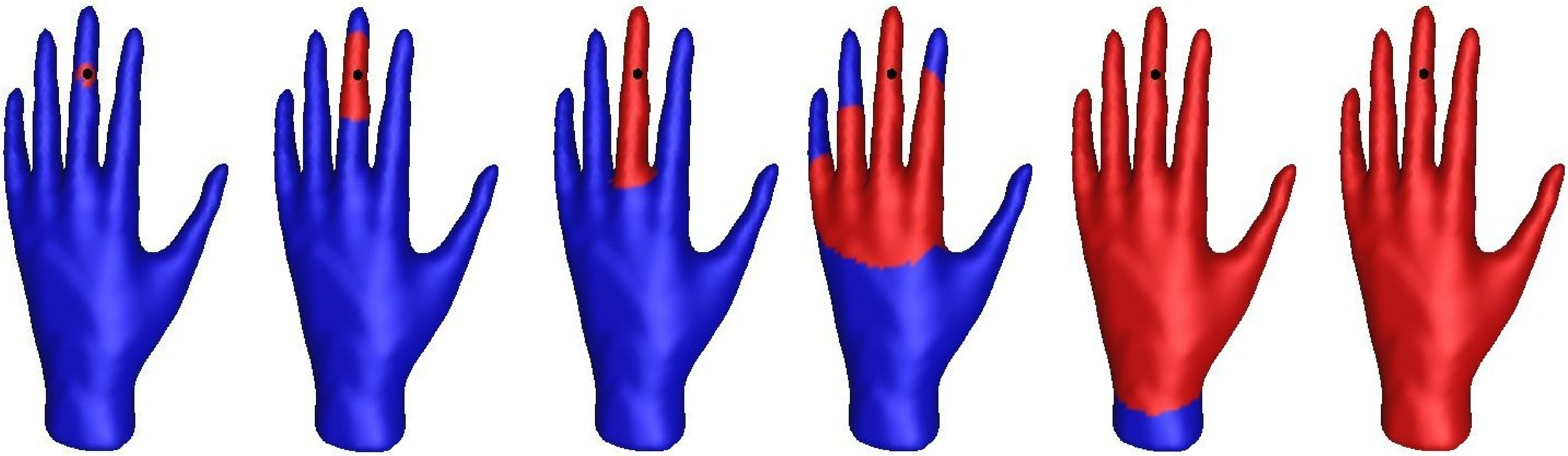
Let $\mathcal{F} = \{\langle \cdot, w \rangle\}_{w \in \mathbb{S}^{d-1}}$, where d is fixed. Then, PHT is injective on the class of semialgebraic sets in $\mathbb{R}^d$.

Corollary: PHT is a sufficient statistic for such sets
$\Rightarrow$ parametric inference



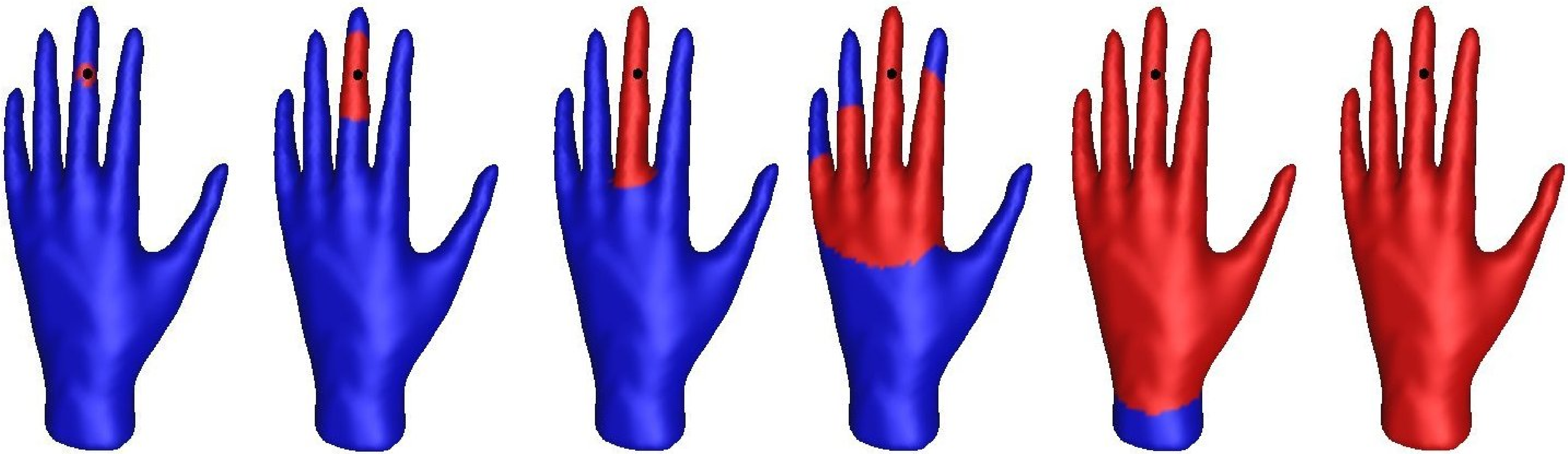
PHT for length spaces

Given a compact length space (X, d_X), take $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$



PHT for length spaces

Given a compact length space (X, d_X), take $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$



Thm (local stability): [Carrière, O., Ovsjanikov 2015]
Let (X, d_X) and (Y, d_Y) be compact length spaces with positive convexity radius ($\varrho(X), \varrho(Y) > 0$). Let $x \in X$ and $y \in Y$. If $\mathrm{d}_{\mathrm{GH}}((X,x),(Y,y)) \leq \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$, then

$$\mathrm{d_b}(\mathrm{dgm}\,\mathrm{d}_X(\cdot,x), \mathrm{dgm}\,\mathrm{d}_Y(\cdot,y)) \leq 20\ \mathrm{d}_{\mathrm{GH}}((X,x),(Y,y)).$$

PHT for length spaces

Given a compact length space (X, d_X), take $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$

Corollary (local stability of PHT):

Let (X, d_X) and (Y, d_Y) be compact length spaces with positive convexity radius $(\varrho(X), \varrho(Y) > 0)$.
If $\mathrm{d}_{\mathrm{GH}}(X, Y) \leq \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$, then

$$\mathrm{d}_{\mathrm{H}}(\mathsf{PHT}(X), \mathsf{PHT}(Y)) \leq 20\ \mathrm{d}_{\mathrm{GH}}((X, x), (Y, y)).$$

Thm (local stability): [Carrière, O., Ovsjanikov 2015]

Let (X, d_X) and (Y, d_Y) be compact length spaces with positive convexity radius $(\varrho(X), \varrho(Y) > 0)$. Let $x \in X$ and $y \in Y$.
If $\mathrm{d}_{\mathrm{GH}}((X, x), (Y, y)) \leq \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$, then

$$\mathrm{d}_{\mathrm{b}}(\mathrm{dgm}\, \mathrm{d}_X(\cdot, x), \mathrm{dgm}\, \mathrm{d}_Y(\cdot, y)) \leq 20\ \mathrm{d}_{\mathrm{GH}}((X, x), (Y, y)).$$

PHT for length spaces

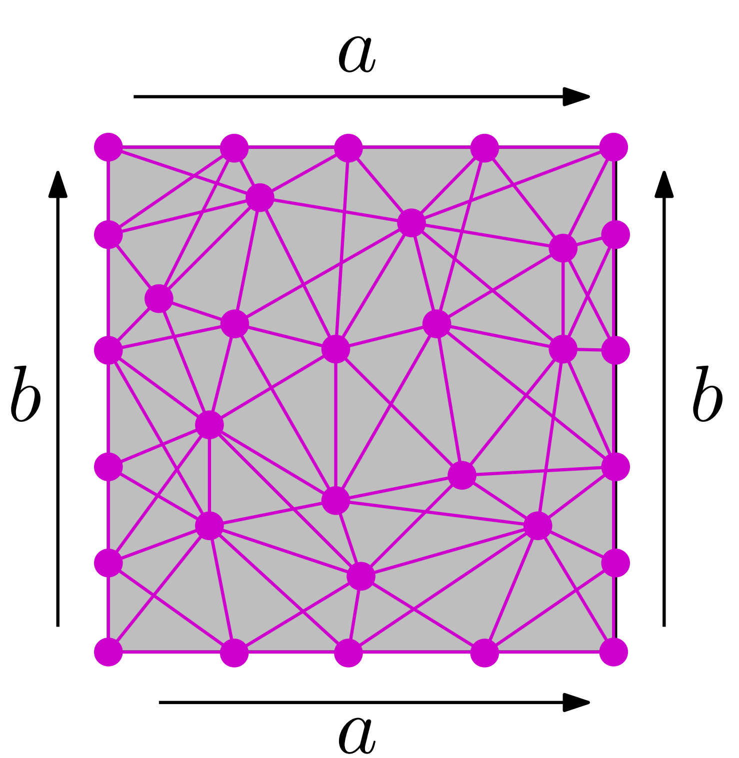
Given a compact length space (X, d_X), take $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$

Corollary (local stability of PHT):

Let (X, d_X) and (Y, d_Y) be compact length spaces with positive convexity radius ($\varrho(X), \varrho(Y) > 0$).

If $\mathrm{d}_{\mathrm{GH}}(X, Y) \leq \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$, then

$$\mathrm{d}_{\mathrm{H}}(\mathsf{PHT}(X), \mathsf{PHT}(Y)) \leq 20\, \mathrm{d}_{\mathrm{GH}}((X, x), (Y, y)).$$



$$\mathrm{d}_{\mathrm{GH}}(T, X) \xrightarrow{\#X \to \infty} 0$$

$\mathrm{d}_{\mathrm{H}}(\mathsf{PHT}_2(T), \mathsf{PHT}_2(X))$ is bounded away from 0

PHT for metric graphs

Focus: compact metric graphs (1-dimensional stratified length spaces)

PHT: $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$, dgm = extended persistence diagram

Thm (global stability): [Dey, Shi, Wang 2015]
For any compact metric graphs X, Y,

$$\mathrm{d_H}(\mathsf{PHT}(X), \mathsf{PHT}(Y)) \leq 18\, \mathrm{d_{GH}}(X, Y).$$

Thm (density): [Gromov]
Compact metric graphs are GH-dense
among the compact length spaces.

PHT for metric graphs

Focus: compact metric graphs (1-dimensional stratified length spaces)

PHT: $\mathcal{F} = \{\mathrm{d}_X(\cdot, x)\}_{x \in X}$, dgm = extended persistence diagram

Thm (global stability): [Dey, Shi, Wang 2015]
For any compact metric graphs X, Y,

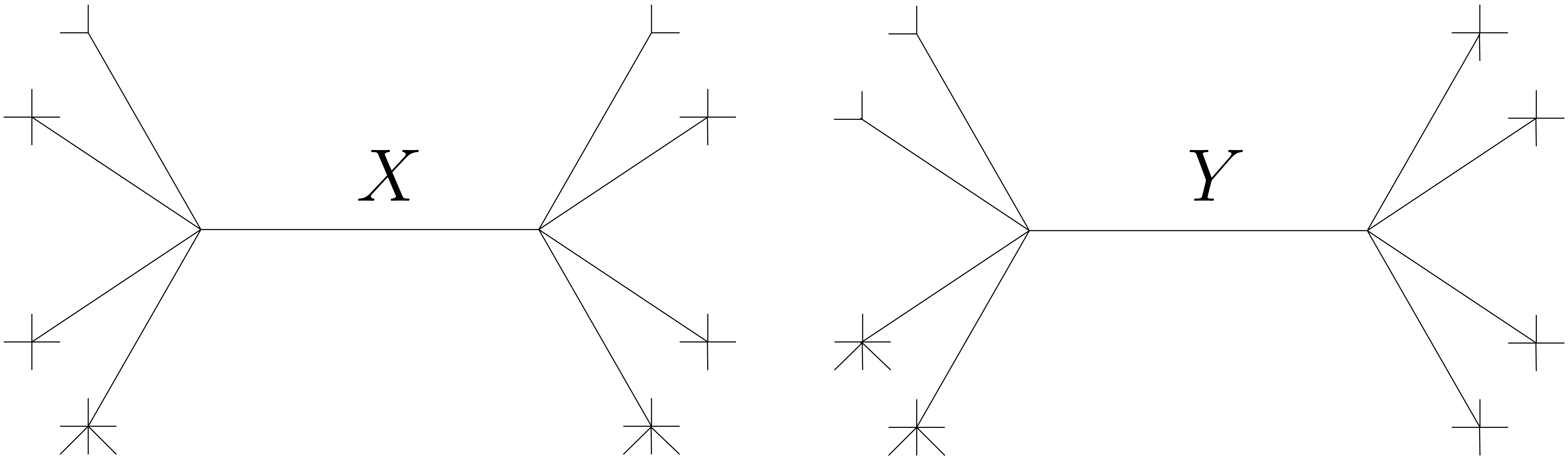
$$\mathrm{d_H}(\mathsf{PHT}(X), \mathsf{PHT}(Y)) \leq 18\, \mathrm{d_{GH}}(X, Y).$$

Thm (density): [Gromov]
Compact metric graphs are GH-dense among the compact length spaces.

Q: injectivity of PHT on metric graphs?

PHT for metric graphs

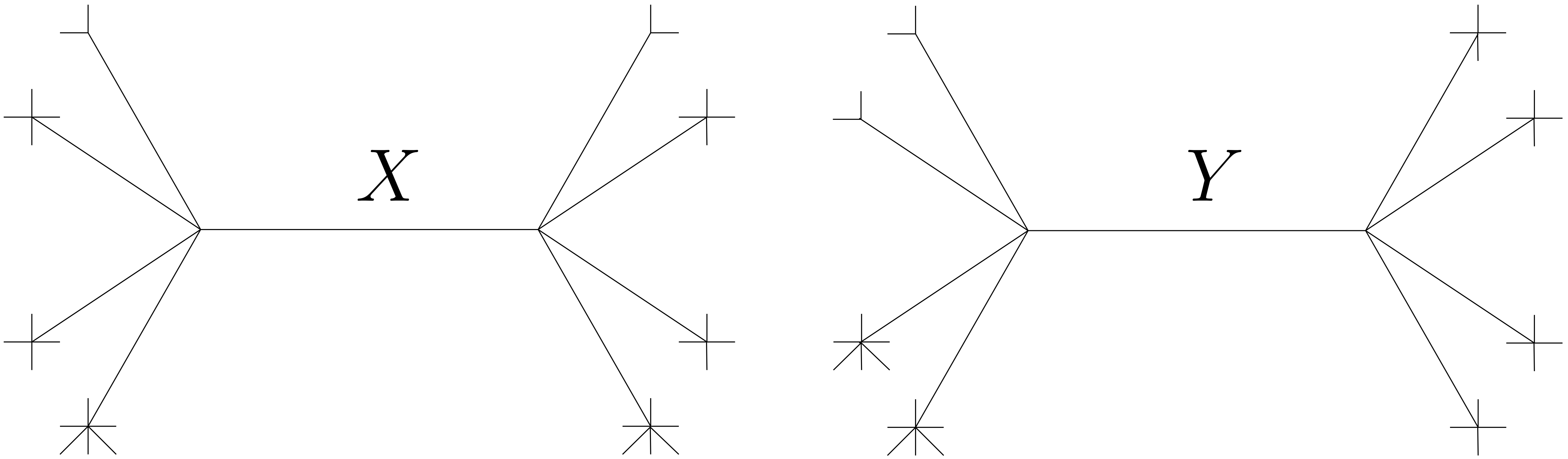
Bad news: PHT is not injective on all compact metric graphs



$$\mathsf{PHT}(X) = \mathsf{PHT}(Y) \text{ while } X \not\simeq Y$$

PHT for metric graphs

Bad news: PHT is not injective on all compact metric graphs



$\mathsf{PHT}(X) = \mathsf{PHT}(Y)$ while $X \not\simeq Y$

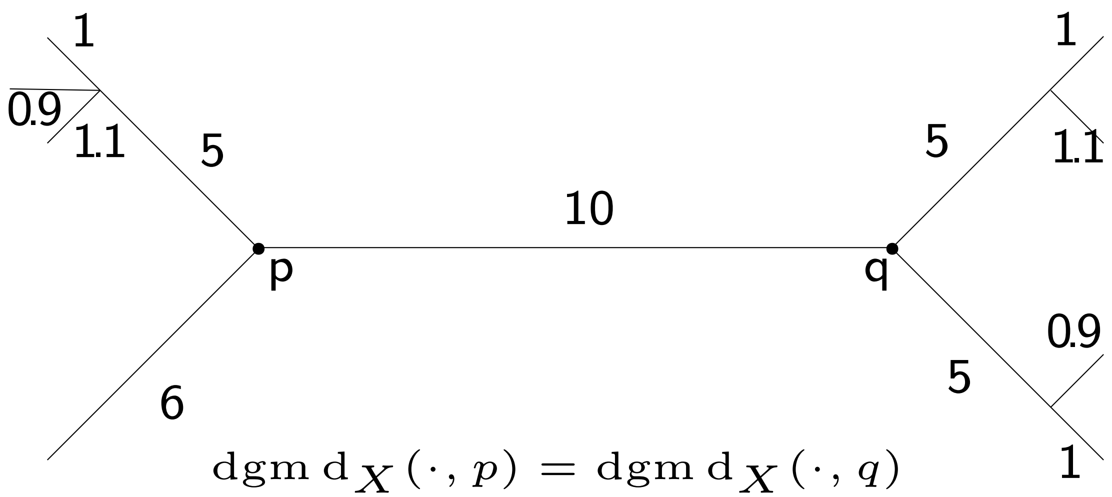
Note: $\mathsf{Aut}(X)$ is non-trivial, hence $\Psi_X : x \mapsto \mathrm{dgm}\, \mathrm{d}_X(\cdot, x)$ is not injective

PHT for metric graphs

Let $\mathrm{Inj}_\Psi = \{X$ compact metric graph s.t. Ψ_X is injective$\}$

Thm 1:
PHT is injective on Inj_Ψ.

Thm 2:
Inj_Ψ is GH-dense among the compact metric graphs.



Note: Ψ_X injective $\underset{\not\Leftarrow}{\Rightarrow}$ $\mathrm{Aut}(X)$ trivial

PHT for metric graphs

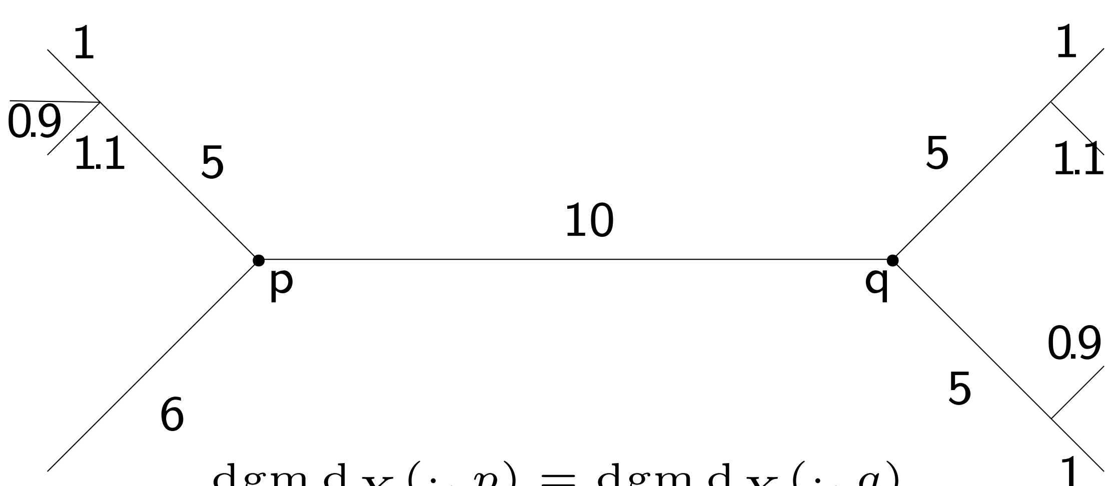
Let $\mathrm{Inj}_\Psi = \{X$ compact metric graph s.t. Ψ_X is injective$\}$

Thm 1:
PHT is injective on Inj_Ψ.

Thm 2:
Inj_Ψ is GH-dense among the compact metric graphs.

+ Gromov's density result

Corollary:
There is a GH-dense subset of the compact length spaces on which PHT is injective.



$\mathrm{dgm}\,\mathrm{d}_X(\cdot, p) = \mathrm{dgm}\,\mathrm{d}_X(\cdot, q)$

Note: Ψ_X injective $\underset{\not\Leftarrow}{\Rightarrow}$ Aut(X) trivial

PHT for metric graphs

Let $\mathrm{Inj}_\Psi = \{X$ compact metric graph s.t. Ψ_X is injective$\}$

+ Gromov's density result

Thm 1:

PHT is injective on Inj_Ψ.

Thm 2:

Inj_Ψ is GH-dense among the compact metric graphs.

Corollary:

There is a GH-dense subset of the compact length spaces on which PHT is injective.

Thm 3:

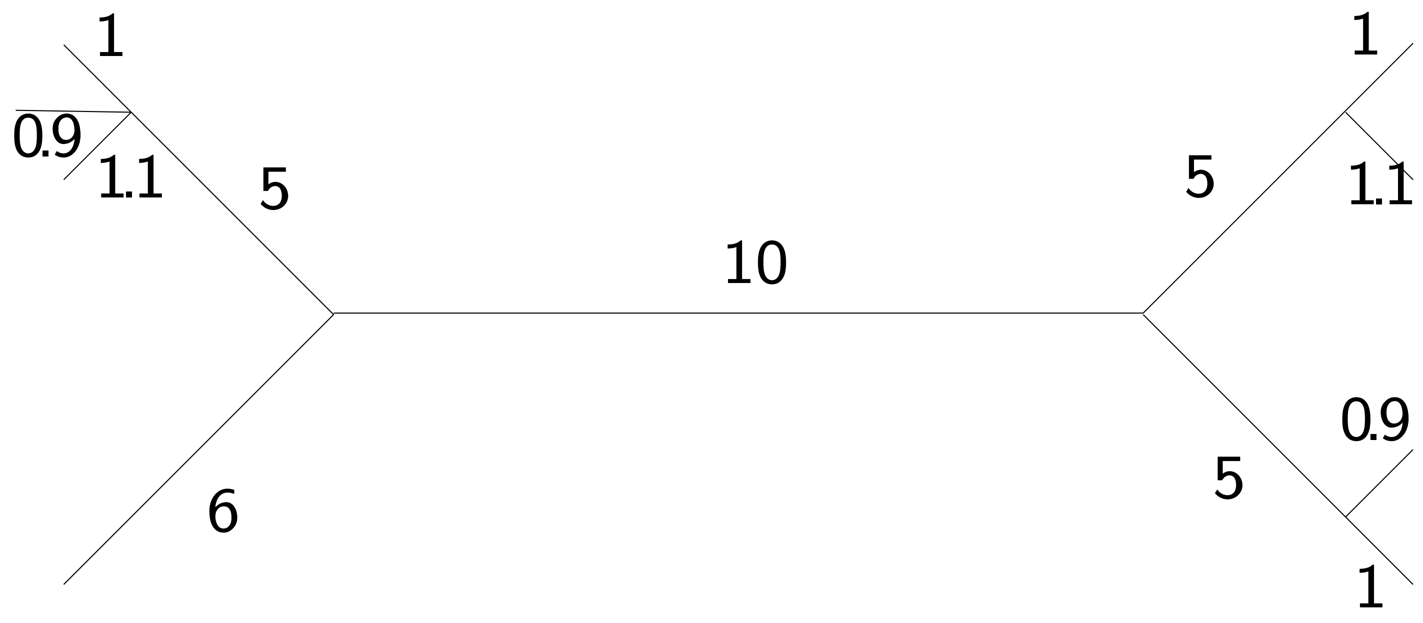
PHT is GH-*locally* injective on compact metric graphs.

Generic injectivity

Generative model:

metric graph $\equiv$ combinatorial graph (V, E) + edge weights $E \to \mathbb{R}_+$

mixture (proba. mass function , proba. measure **with density** on $\mathbb{R}_+^{|E|}$)



Generic injectivity

Generative model:

metric graph $\equiv$ combinatorial graph (V, E) + edge weights $E \to \mathbb{R}_+$

mixture (proba. mass function , proba. measure **with density** on $\mathbb{R}_+^{|E|}$)

Thm 4:

Under this model, there is a full-measure subset of the metric graphs on which PHT is injective.

Generic injectivity

Generative model:

metric graph $\equiv$ combinatorial graph (V, E) + edge weights $E \to \mathbb{R}_+$

mixture (proba. mass function , proba. measure **with density** on $\mathbb{R}_+^{|E|}$)

Thm 4:
Under this model, there is a full-measure subset of the metric graphs on which PHT is injective.

Questions:

- is PHT a sufficient statistic for metric graphs?
- are finitely many basepoints enough? algorithm?
- what about higher-dimensional stratified spaces?

Proof outline for Thm 1

Let $\text{Inj}_\Psi = \{X$ compact metric graph s.t. Ψ_X is injective$\}$

+ Gromov's density result

Thm 1:

PHT is injective on Inj_Ψ.

Thm 2:

Inj_Ψ is GH-dense among the compact metric graphs.

Corollary:

There is a GH-dense subset of the compact length spaces on which PHT is injective.

Thm 3:

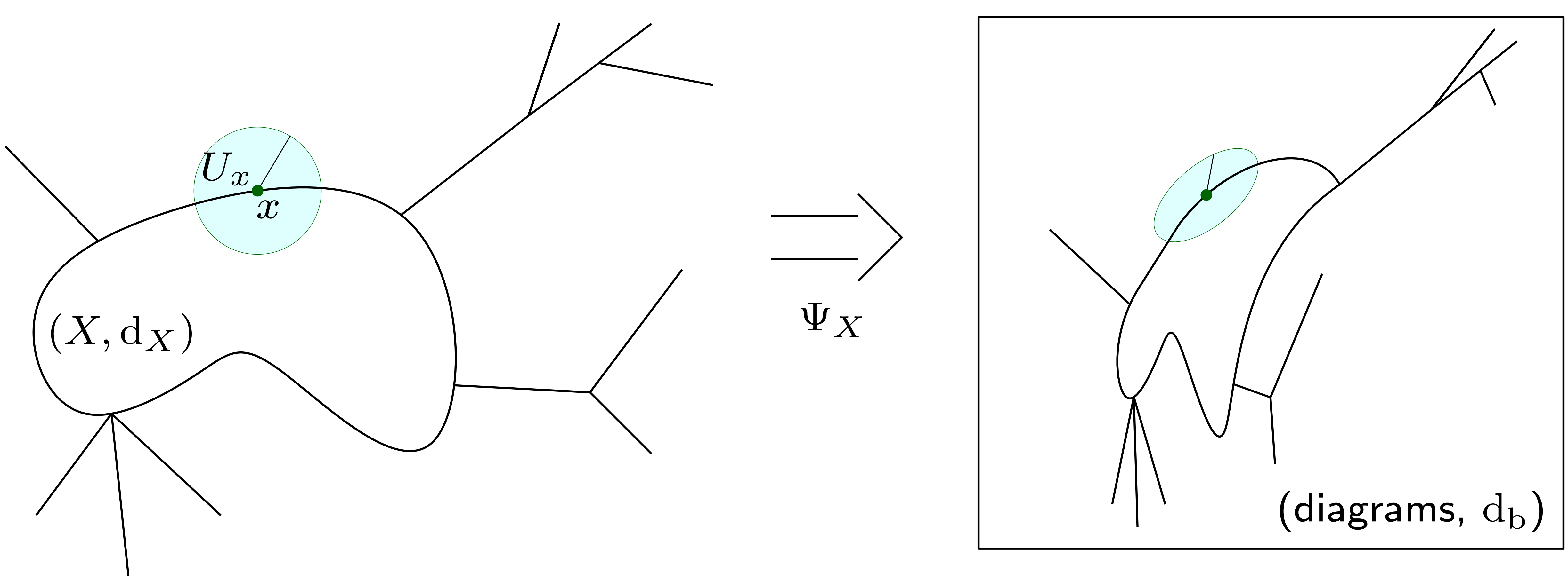
PHT is GH-*locally* injective on compact metric graphs.

Proof outline for Thm 1

Prop:

If X is not a circle, then Ψ_X is a *local* isometry:

$$\forall x \; \exists U_x \; \forall y \in U_x \; \mathrm{d}_X(x,y) = \mathrm{d}_{\mathrm{b}}(\Psi_X(x), \Psi_X(y))$$



Proof outline for Thm 1

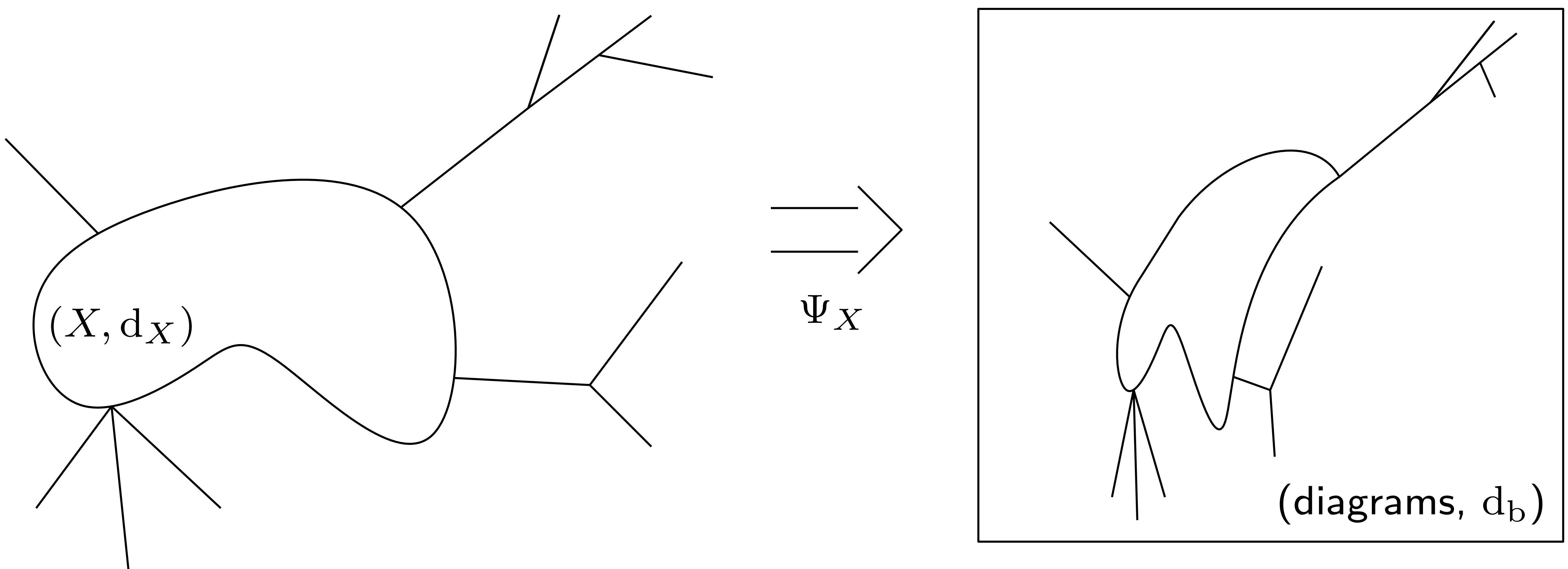
Prop:

If X is not a circle, then Ψ_X is a *local* isometry:

$$\forall x \; \exists U_x \; \forall y \in U_x \; \mathrm{d}_X(x,y) = \mathrm{d}_\mathrm{b}(\Psi_X(x), \Psi_X(y))$$

Corollary:

If Ψ_X is injective, then Ψ_X is a (global) isometry from (X, d_X) to $(\mathsf{PHT}(X), \hat{\mathrm{d}}_\mathrm{b})$.



Proof outline for Thm 2

Let $\mathsf{Inj}_\Psi = \{X$ compact metric graph s.t. Ψ_X is injective$\}$

Thm 1:

PHT is injective on Inj_Ψ.

Thm 2:

Inj_Ψ is GH-dense among the compact metric graphs.

+ Gromov's density result

Corollary:

There is a GH-dense subset of the compact length spaces on which PHT is injective.

Thm 3:

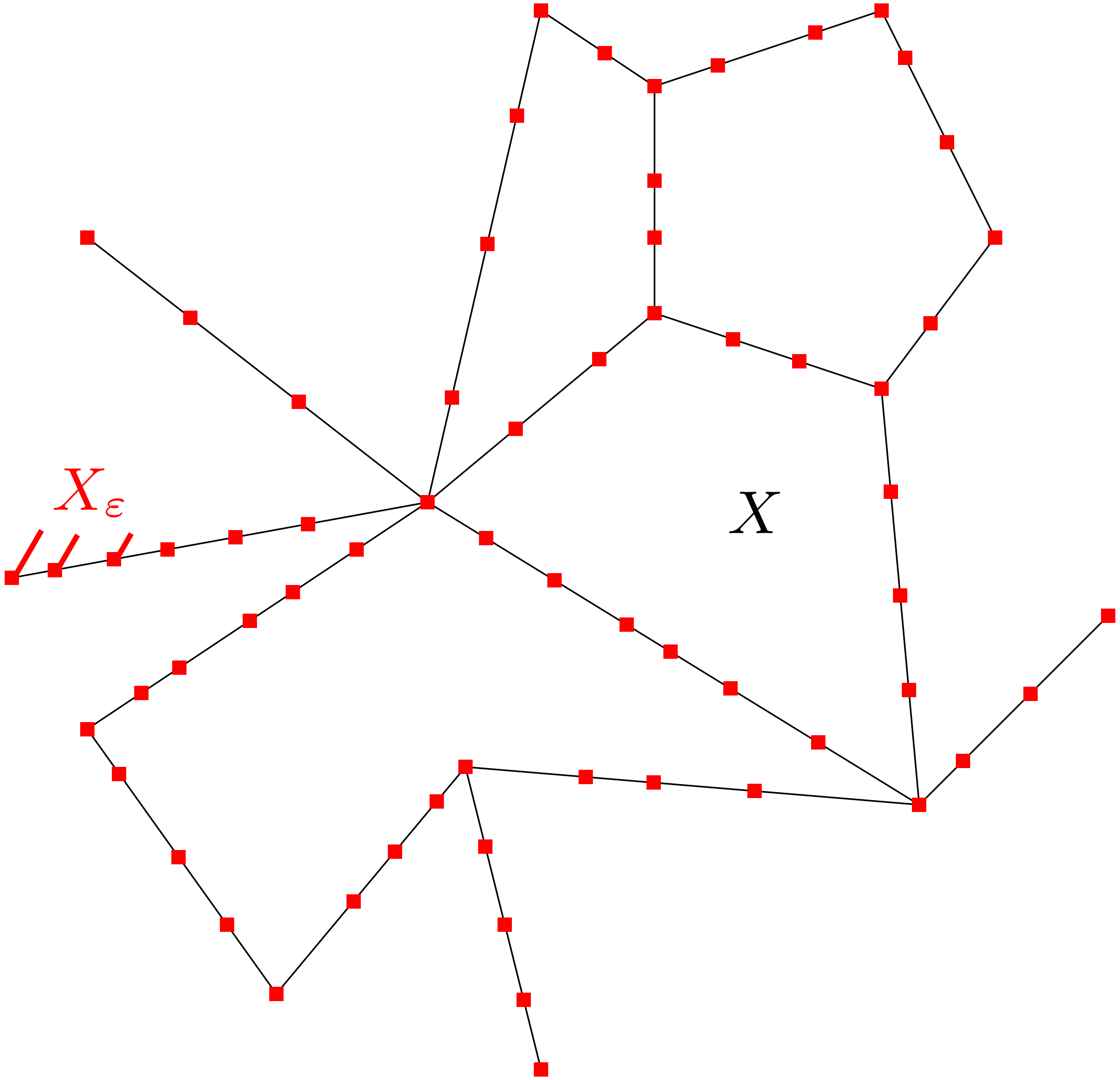
PHT is GH-*locally* injective on compact metric graphs.

Proof outline for Thm 2

Given (X, d_X), for any $\varepsilon > 0$ build an ε-approximation $(X_\varepsilon, \mathrm{d}_{X_\varepsilon})$ in d_{GH}

Break symmetries by **cactification**:

- subdivide edges
- add hanging branches (*thorns*) with distinct lengths

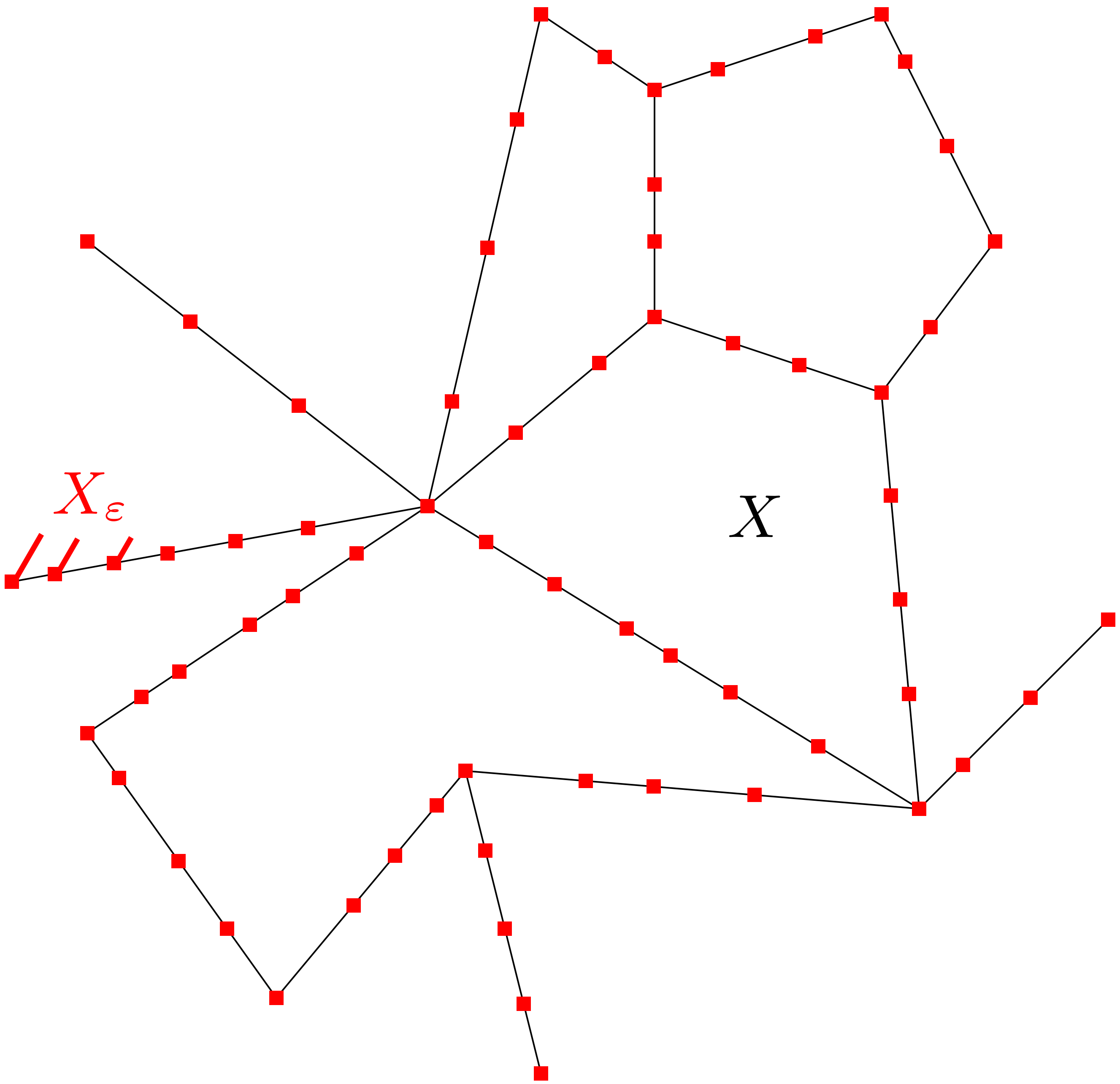


Proof outline for Thm 2

Given (X, d_X), for any $\varepsilon > 0$ build an ε-approximation $(X_\varepsilon, \mathrm{d}_{X_\varepsilon})$ in d_{GH}

Break symmetries by **cactification**:

- subdivide edges
- add hanging branches (*thorns*) with distinct lengths



$\rightarrow$ $(X_\varepsilon, \mathrm{d}_{X_\varepsilon})$ parametrized by distances to thorn bases and tips

$\rightarrow$ these distances appear in the persistence diagrams

Proof outline for Thm 3

Let $\text{Inj}_\Psi = \{X$ compact metric graph s.t. Ψ_X is injective$\}$

+ Gromov's density result

Thm 1:

PHT is injective on Inj_Ψ.

Thm 2:

Inj_Ψ is GH-dense among the compact metric graphs.

Corollary:

There is a GH-dense subset of the compact length spaces on which PHT is injective.

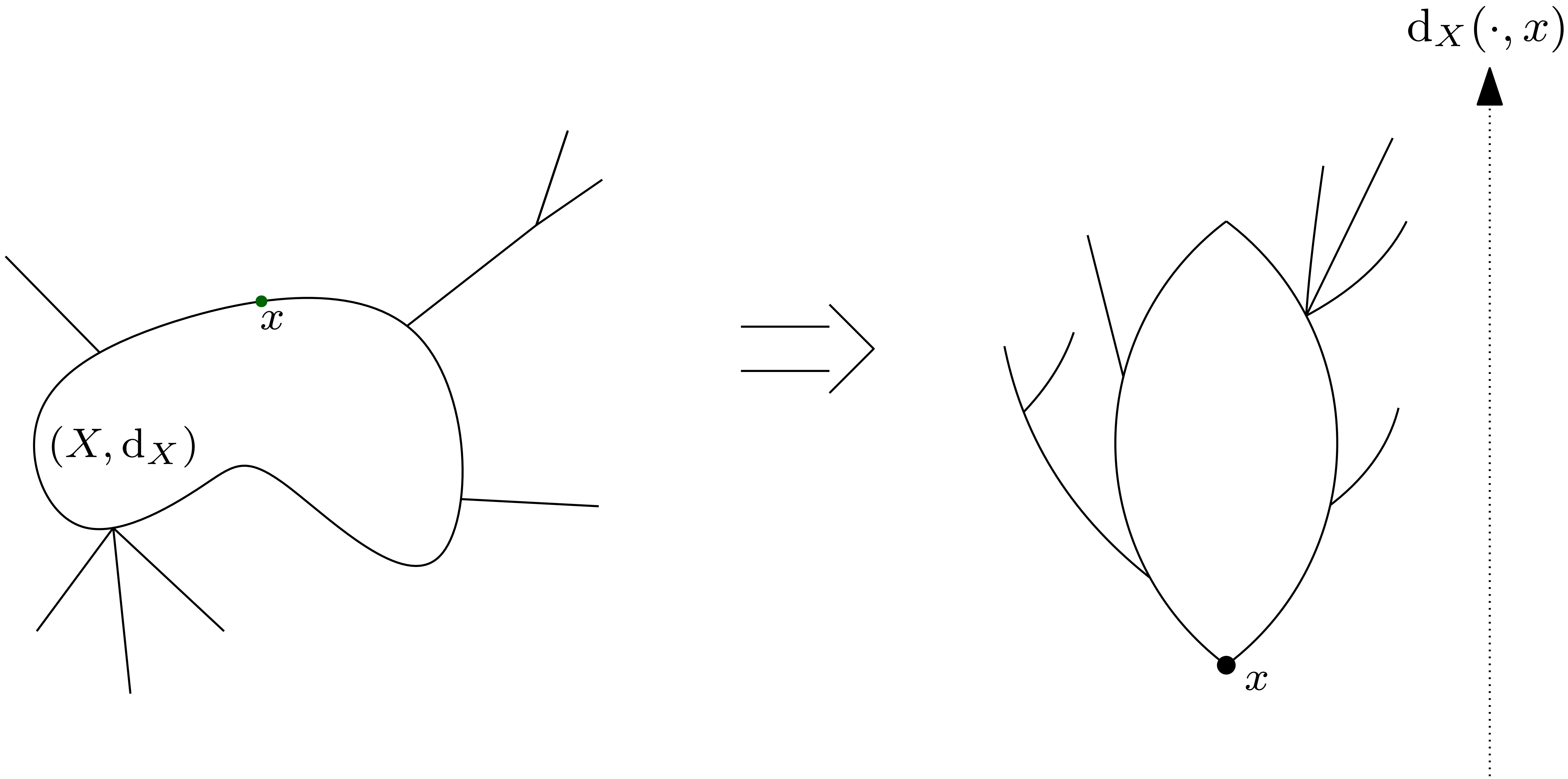
Thm 3:

PHT is GH-*locally* injective on compact metric graphs.

Proof outline for Thm 3

Prop:

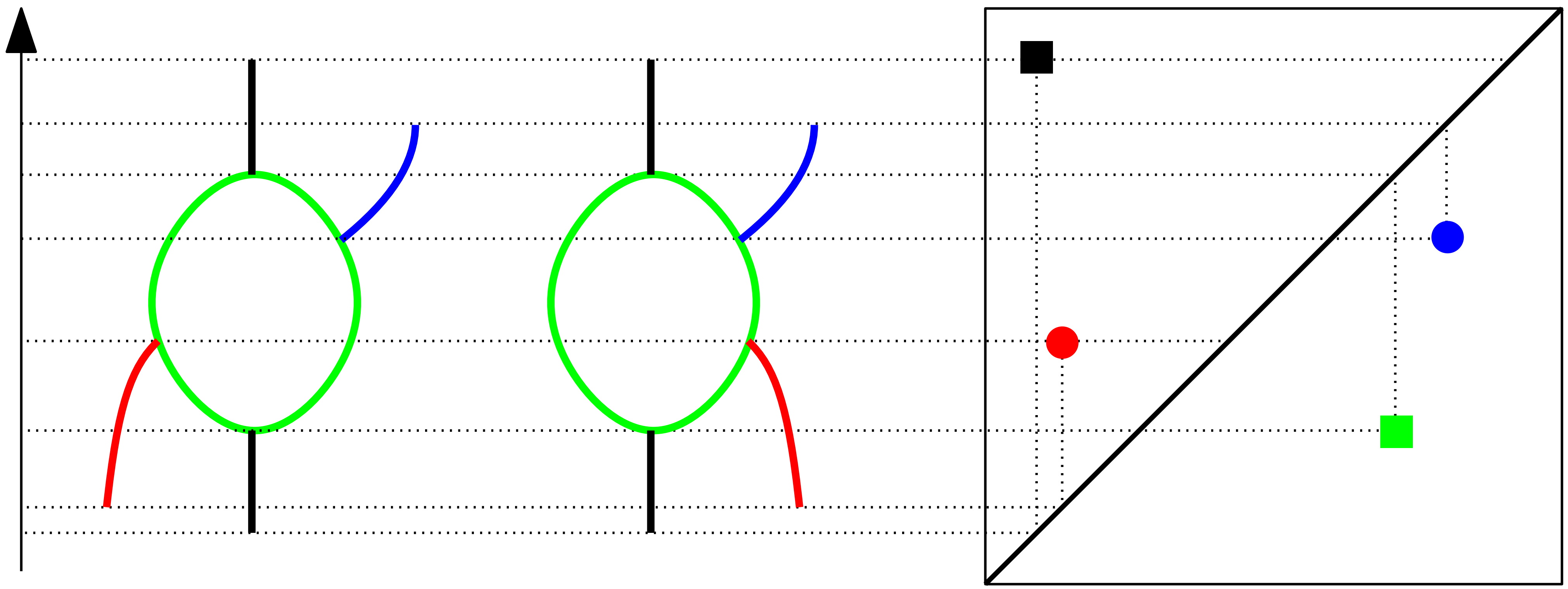
The map $(X, \mathrm{d}_X, x) \mapsto R_{\mathrm{d}_X(\cdot,x)}$ is injective.



Proof outline for Thm 3

Prop:
The map $(X, \mathrm{d}_X, x) \mapsto R_{\mathrm{d}_X(\cdot,x)}$ is injective.

Thm: [Carrière, O. 2017]
The map $R_f \mapsto \mathrm{dgm}\, f$ is GH-*locally* injective.



Generic injectivity

Generative model:

metric graph $\equiv$ combinatorial graph (V, E) + edge weights $E \to \mathbb{R}_+$

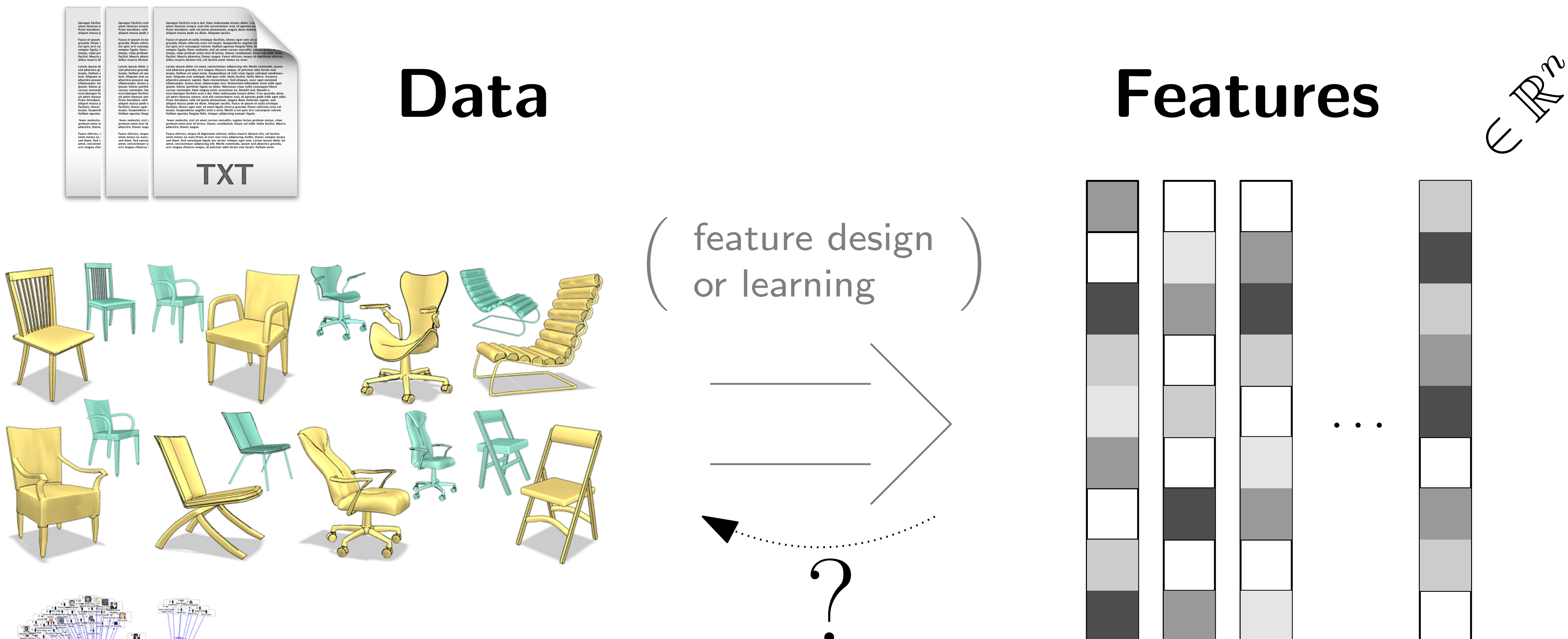
mixture (proba. mass function , proba. measure **with density** on $\mathbb{R}_+^{|E|}$)

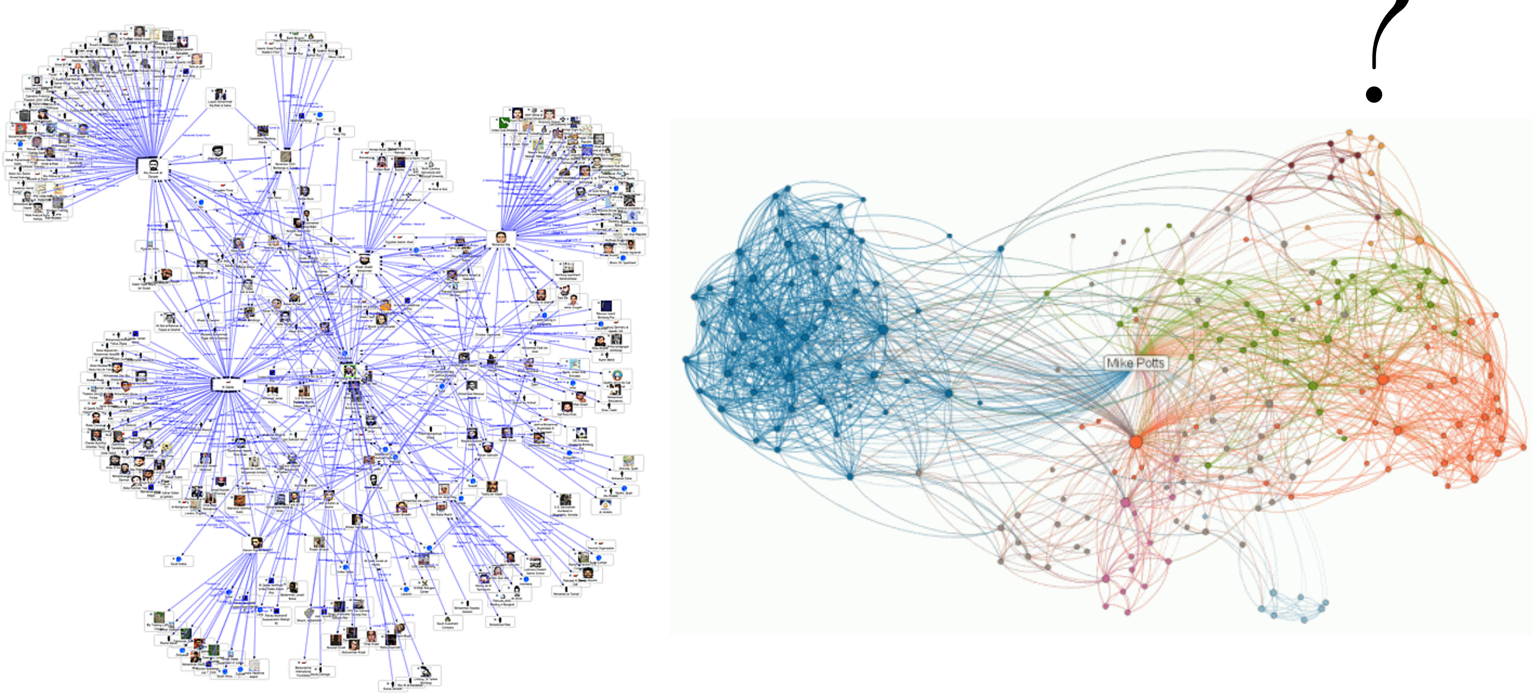
Thm 4:
Under this model, there is a full-measure subset of the metric graphs on which PHT is injective.

Proof outline:

- for (almost) any fixed combinatorial graph G, Ψ_G is *generically* injective.
- deal with exceptions (e.g. linear graphs) explicitly

The preimage problem in the data Sciences





bag of words, word2vec

shape contexts, heat kernels

node2vec, Laplacian fact., rand. walks

dim. reduction, auto-encoders, etc.