Geometry and Topology of Data
ICERM, December 2017

Inverse problems in TDA
Focus on metric graphs

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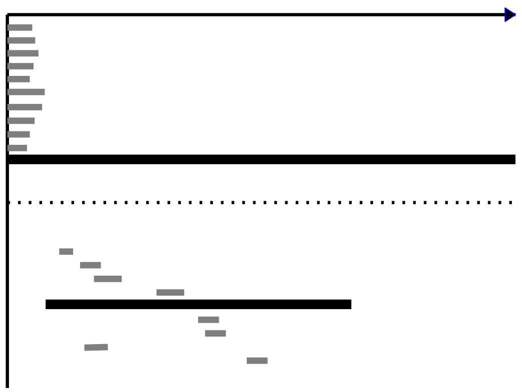
Inria

— joint work with Elchanan (Isaac) Solomon (Brown University)

Persistence diagrams as descriptors for data

Data $\Longrightarrow$ **Descriptor**

(TDA)



- genericity
- stability
- invariance
- $\dots$

Persistence diagrams as descriptors for data

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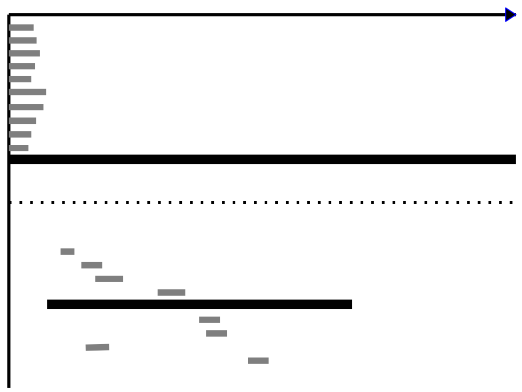
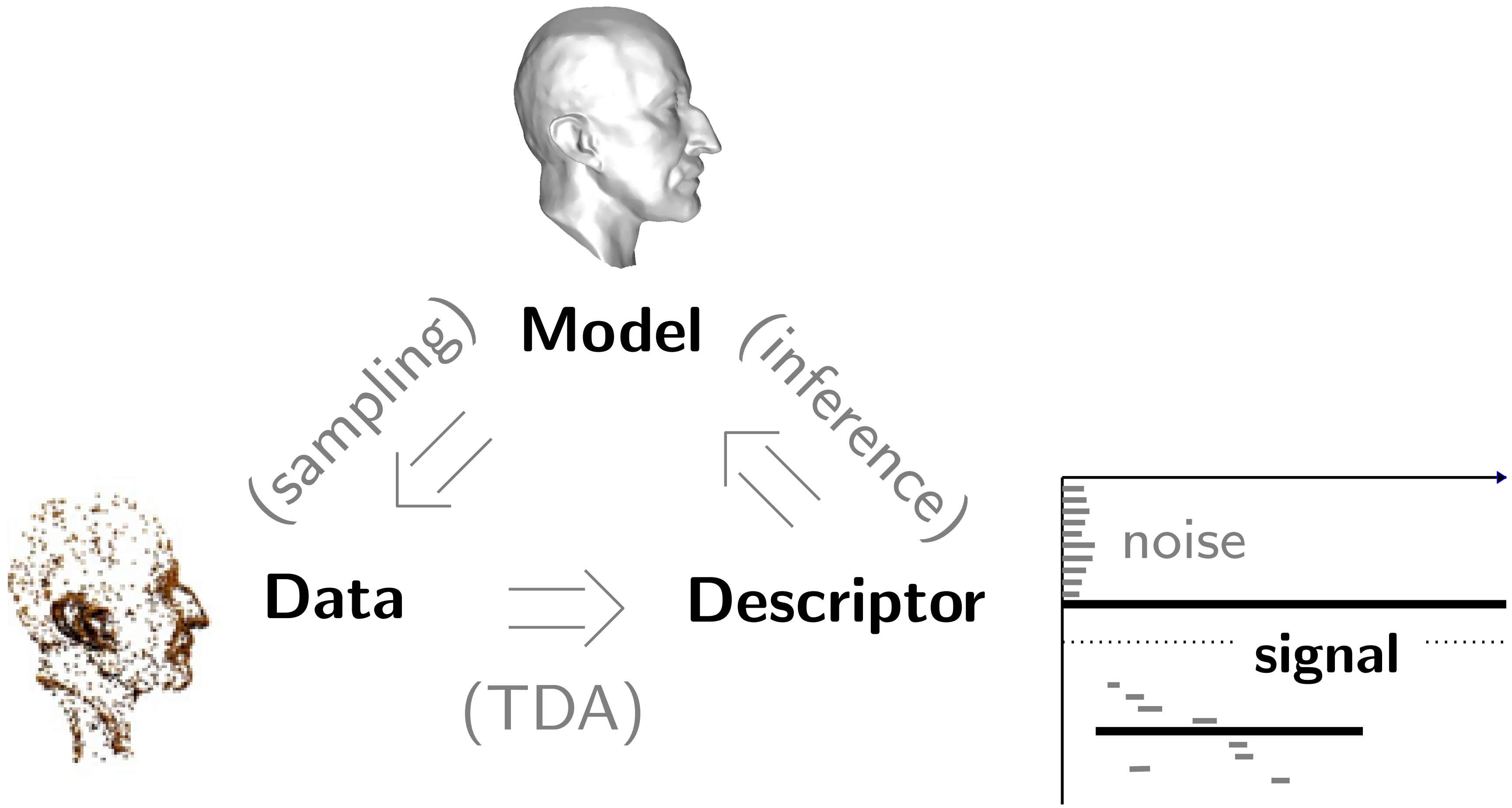
(TDA)



- genericity
- stability
- invariance
- ...

autoencoders!

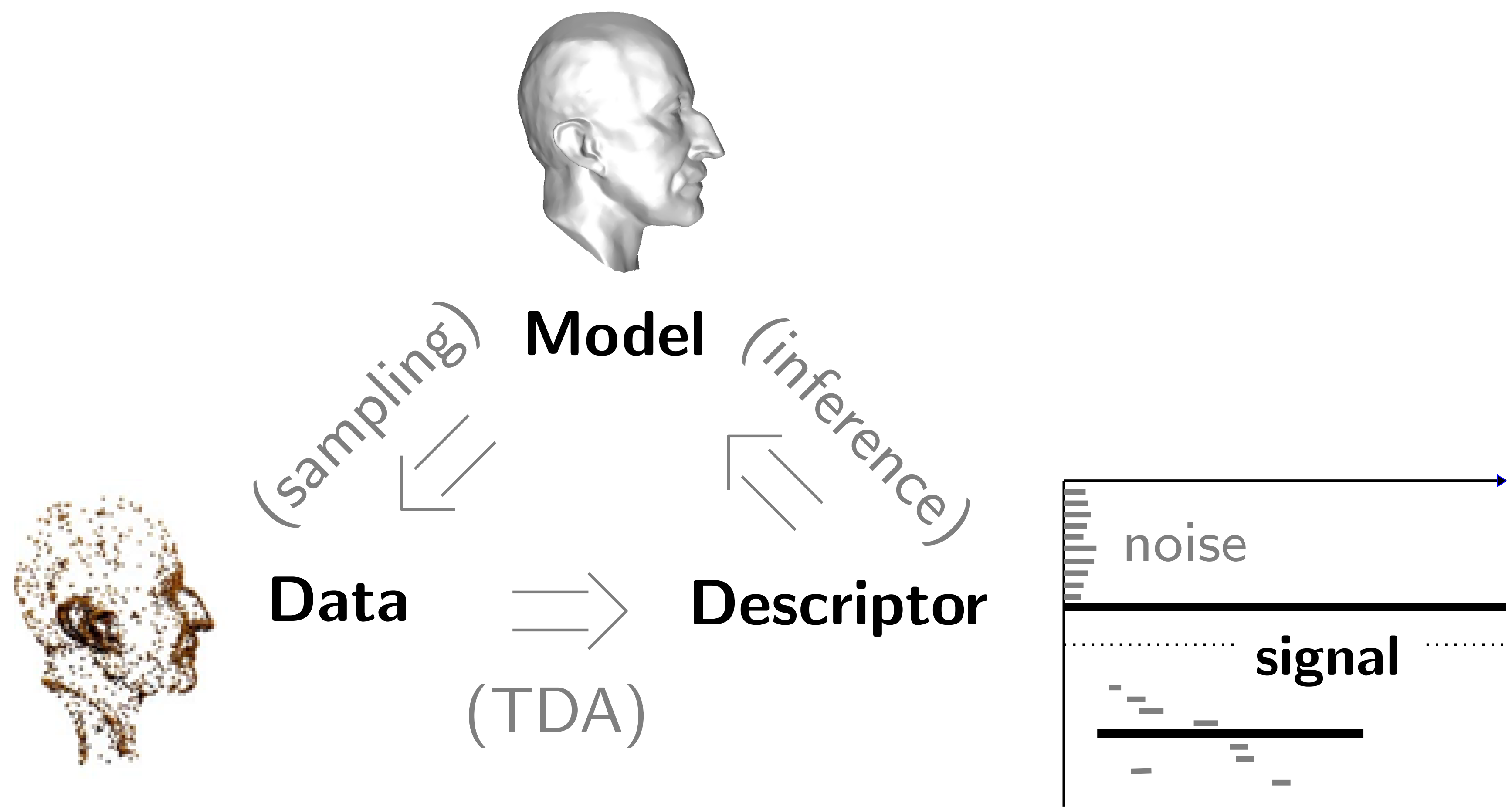
Persistence diagrams as descriptors for data



Challenges:

- signal vs noise discrimination
- model inference
- hypothesis testing
- ...

Persistence diagrams as descriptors for data

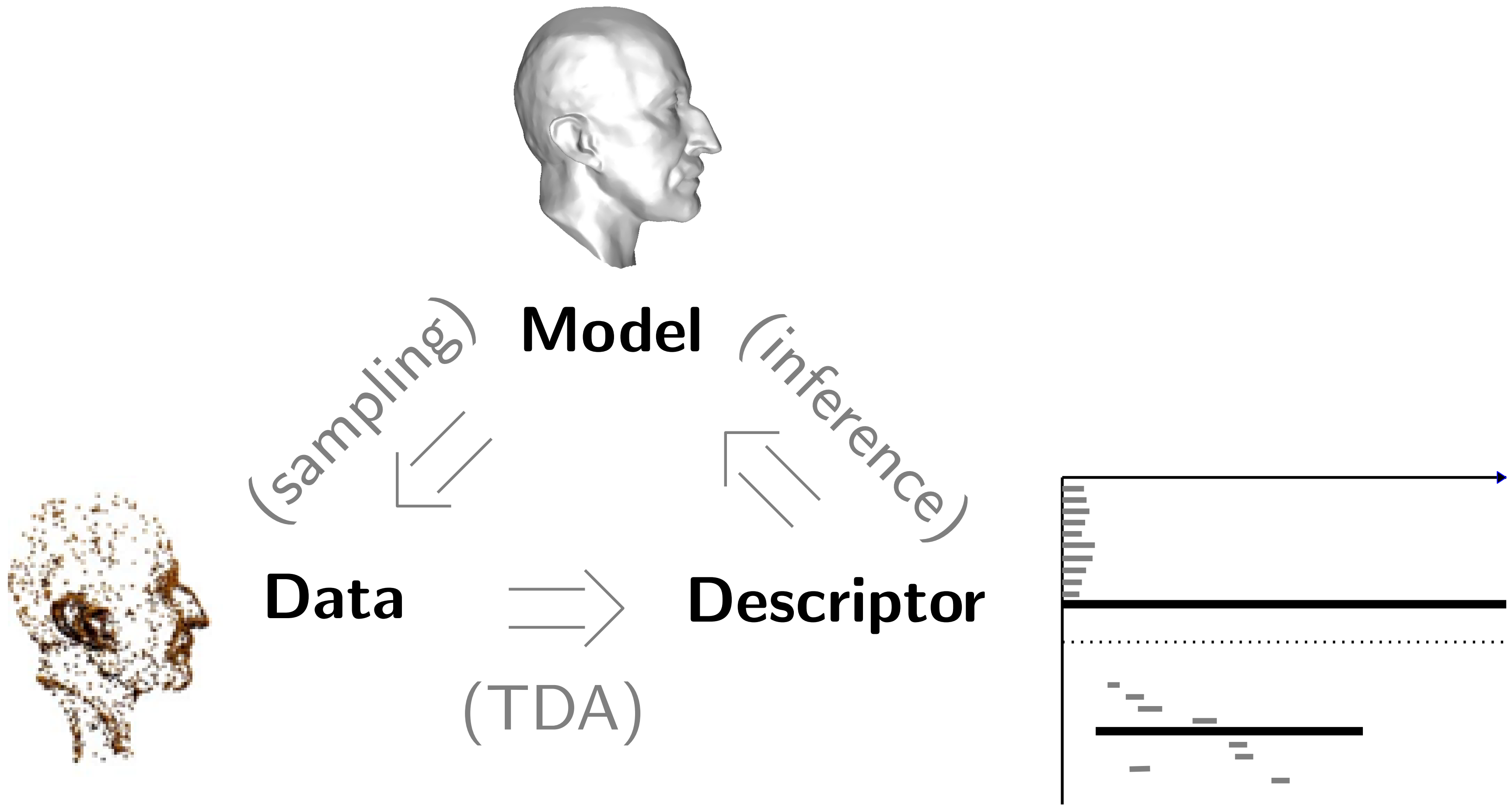


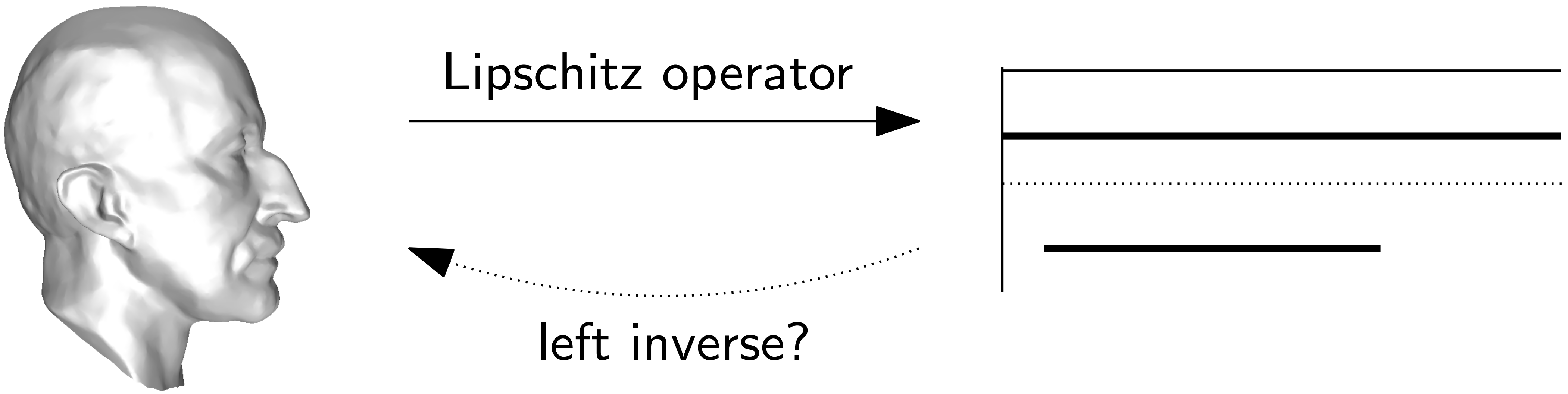
Challenges:

- signal vs noise discrimination
- model inference
- hypothesis testing
- ...

model uniqueness?

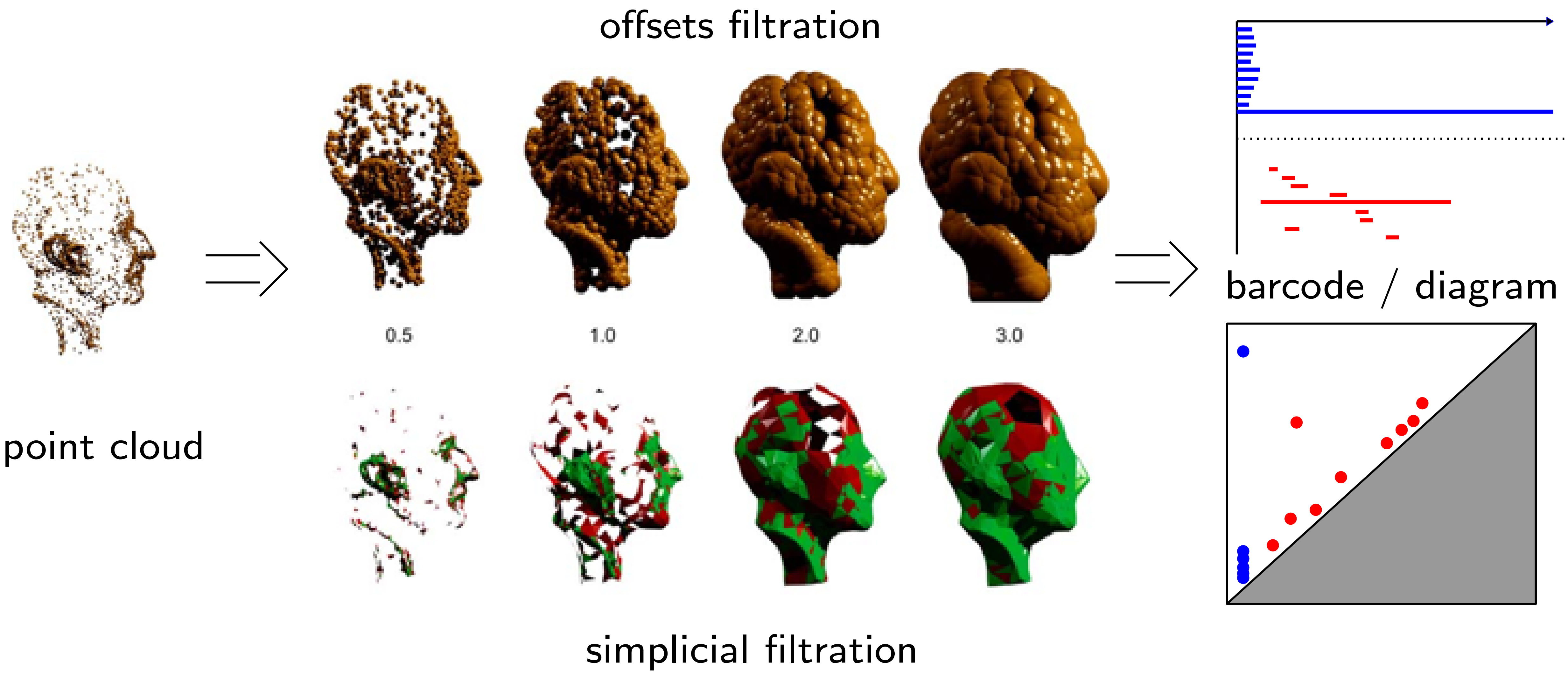
Persistence diagrams as descriptors for data





Lack of injectivity in general

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



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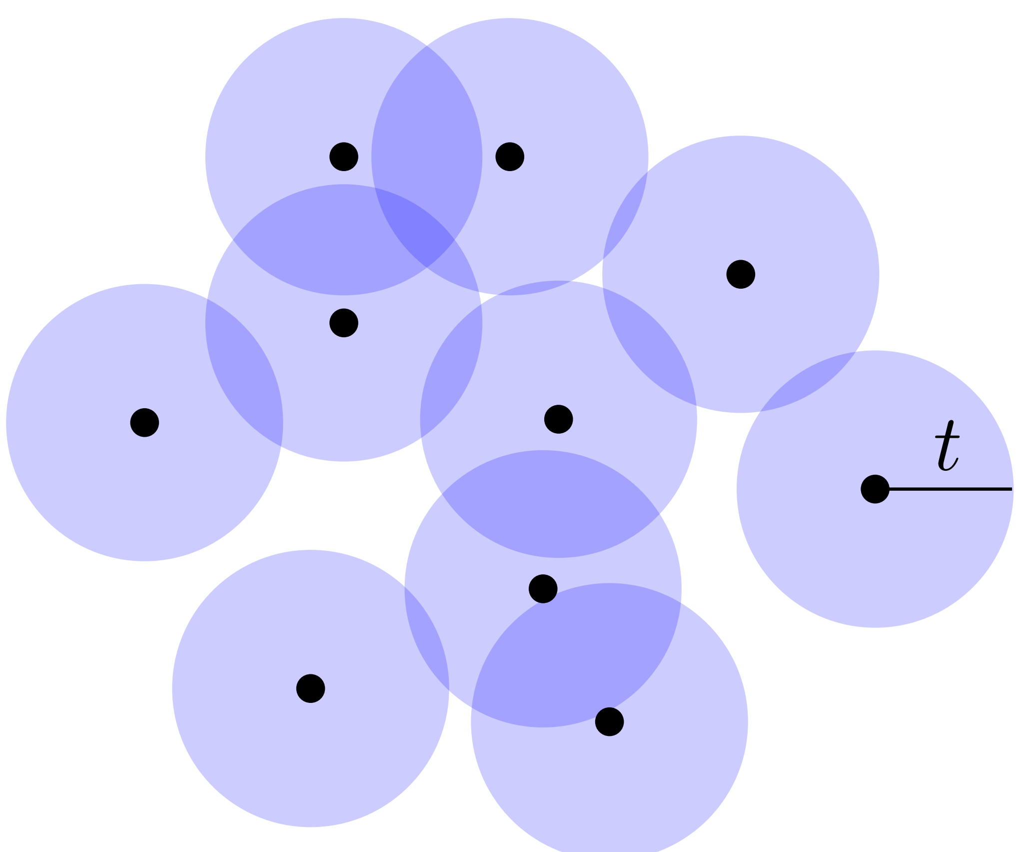
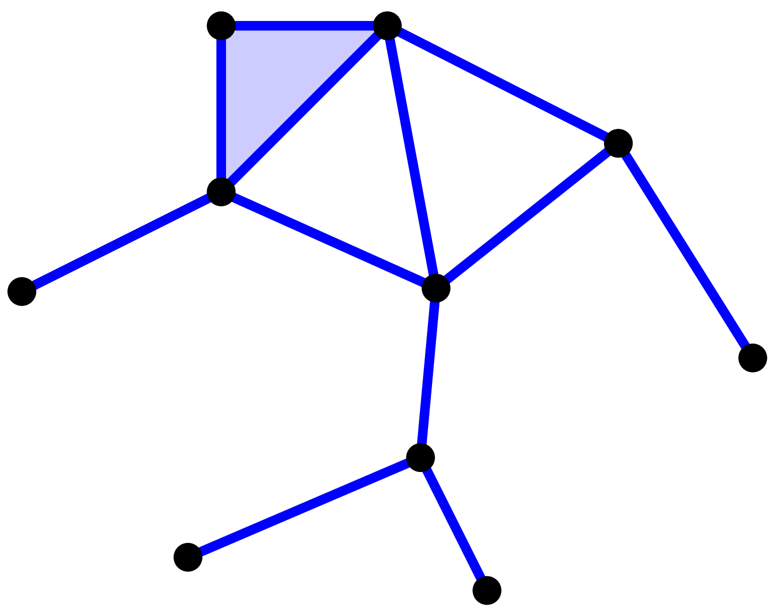
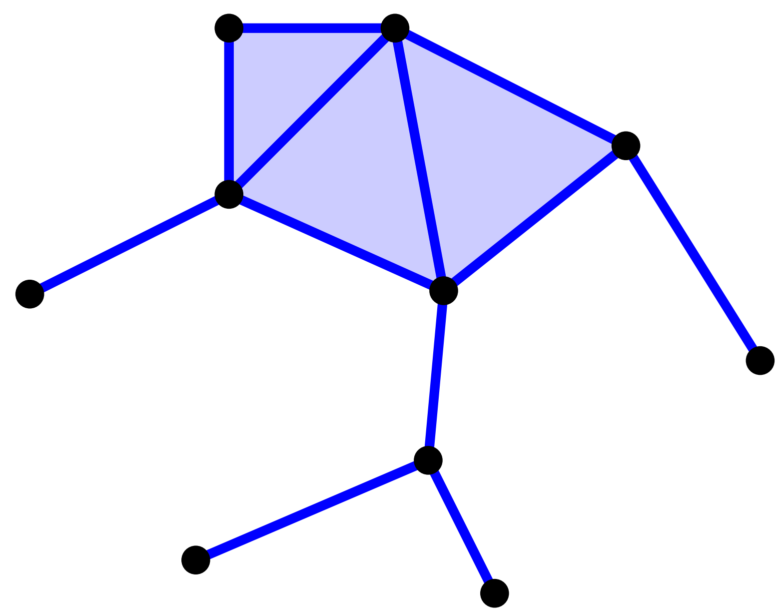




$C_t(X, d_X)$



$R_{2t}(X, d_X)$

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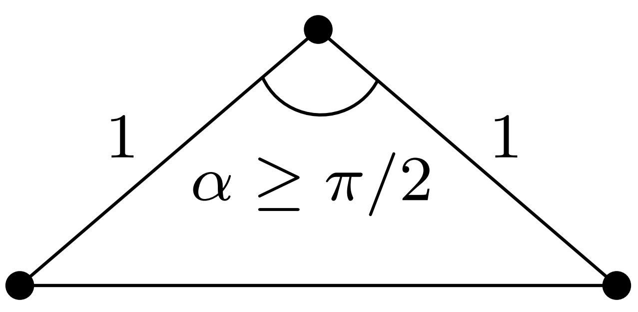


$$\mathrm{dgm}\, \mathcal{C}(P, \ell_2) = \{(0, +\infty)\} \sqcup \{(0, \tfrac{1}{2})\} \sqcup \{(0, \tfrac{1}{2})\}$$

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

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

Lack of injectivity in general

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

Prop: [Folklore]
For any *metric tree* (X, d_X):

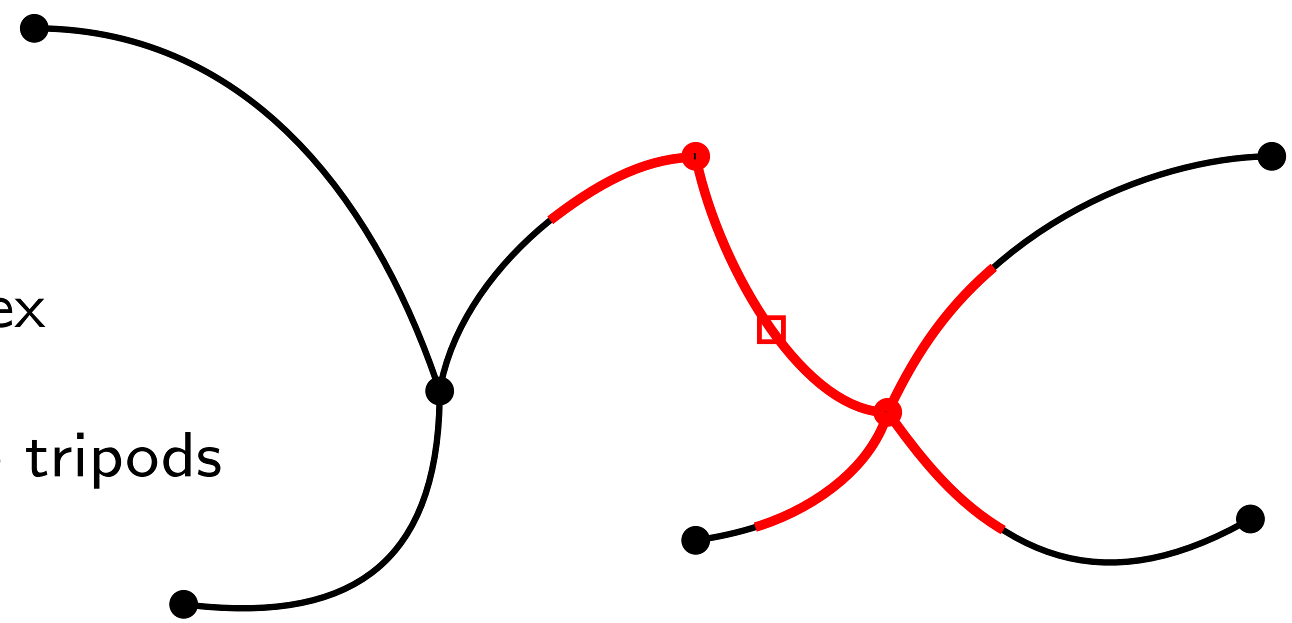
$$\mathrm{dgm}\, \mathcal{R}(X, \mathrm{d}_X) = \mathrm{dgm}\, \mathcal{C}(X, \mathrm{d}_X) = \{(0, +\infty)\}$$

$\Rightarrow$ no information on the metric

X is 0-hyperbolic

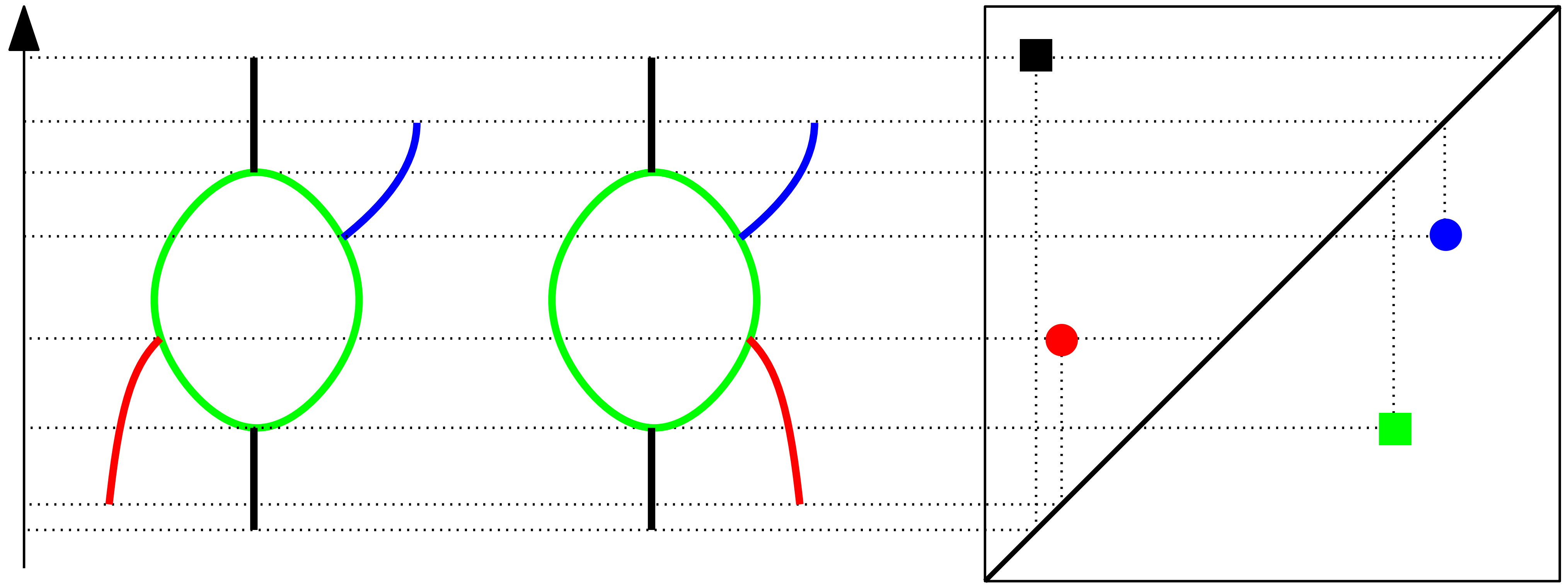
$\Rightarrow$ metric balls are convex

$\Rightarrow$ geodesic triangles are tripods



Lack of injectivity in general

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



$\Rightarrow$ Reeb graphs are indistinguishable from their diagrams

Lack of injectivity in general

- 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,

$$\mathrm{dgm}\, f \circ h = \mathrm{dgm}\, f$$

$\Rightarrow$ Persistence is invariant under reparametrizations

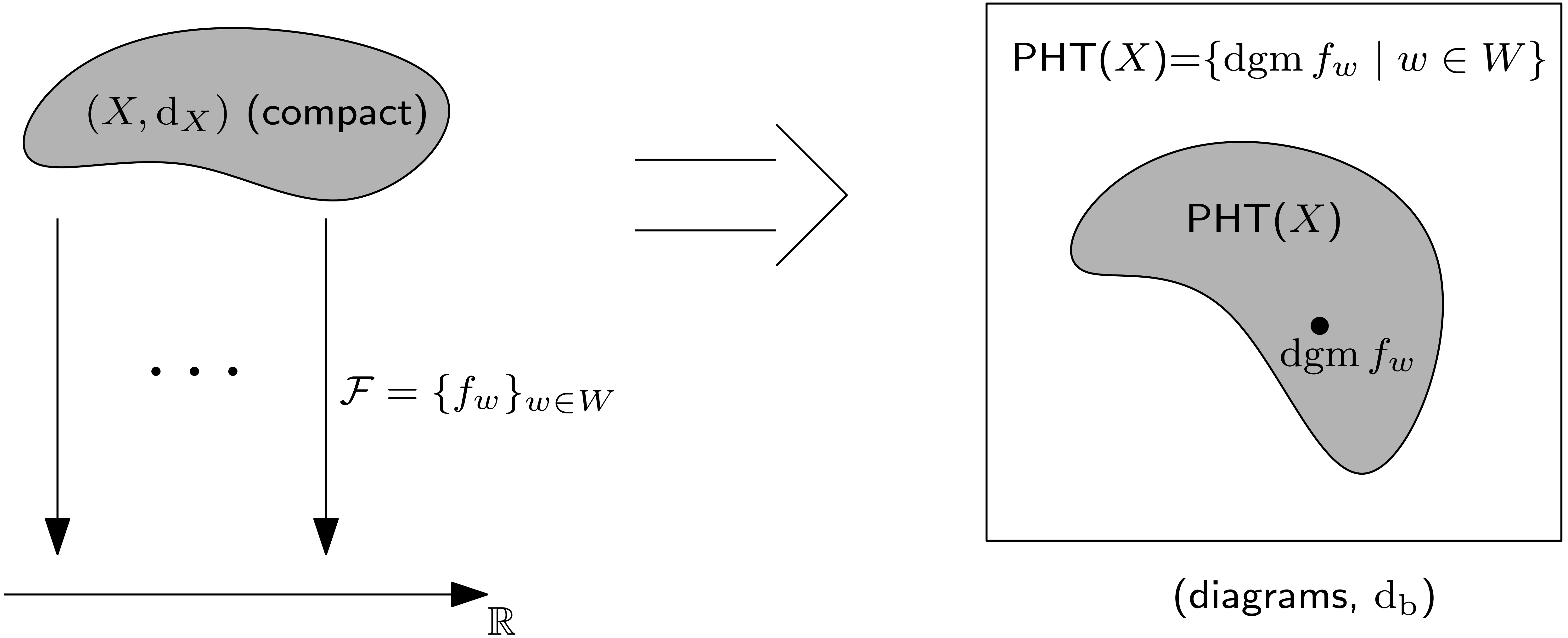
Lack of injectivity in general

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

possible solutions:

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

Persistent Homology Transform (PHT)



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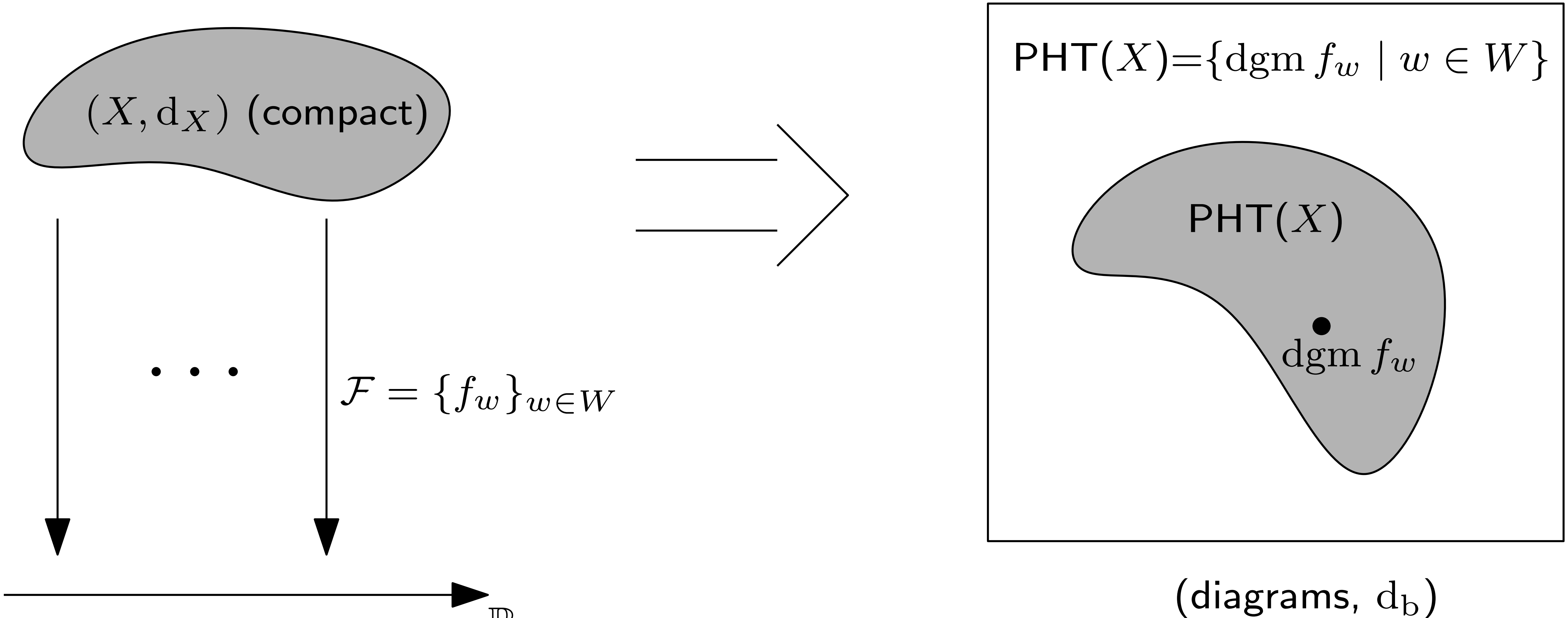
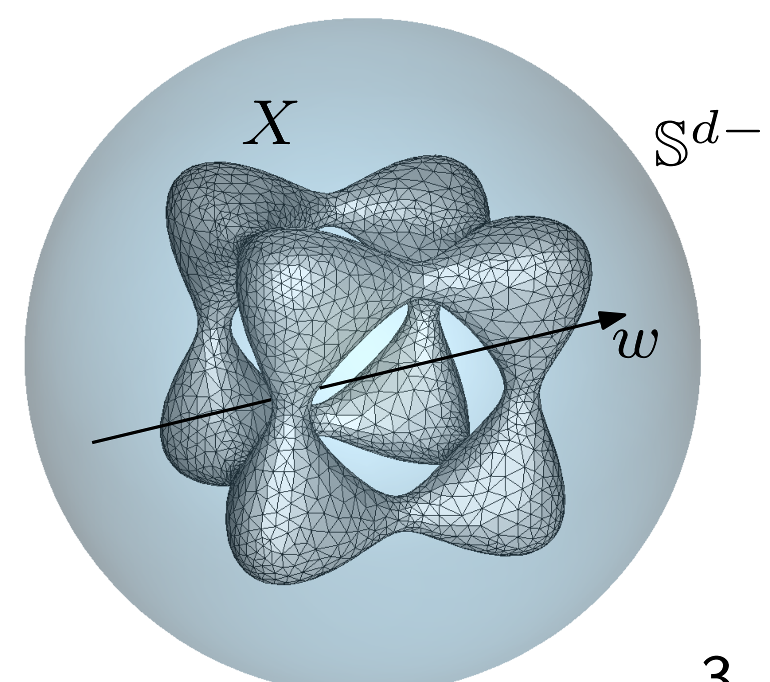


Thm: [Turner, Mukherjee, Boyer 2014]

Let $\mathcal{F} = \{\langle \cdot, w \rangle\}_{w \in \mathbb{S}^{d-1}}$, where $d = 2, 3$ is fixed. Then, PHT is injective on the set of linear embeddings of compact simplicial complexes in $\mathbb{R}^d$.

Extension: [Turner et al., in progress]

True for arbitrary d and semialgebraic compact sets.



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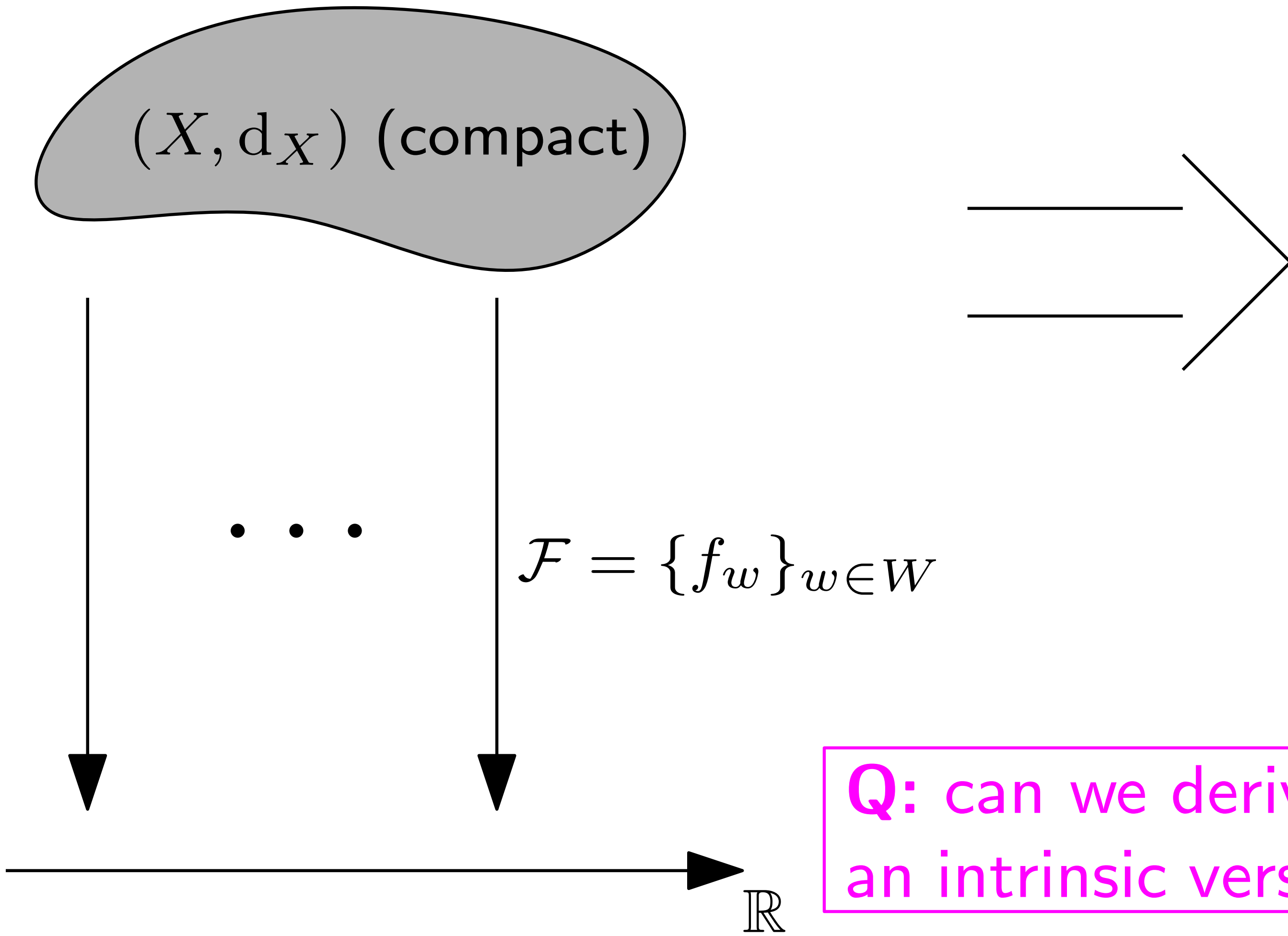

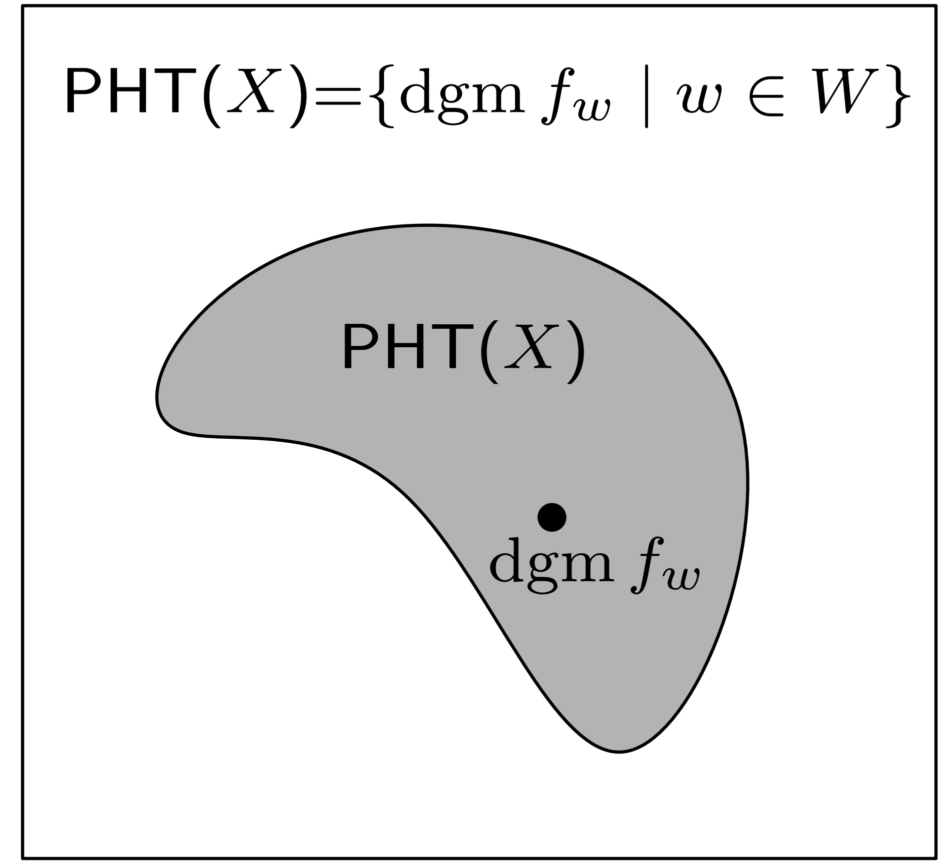

Q: can we derive an intrinsic version?

(diagrams, $\mathrm{d_b}$)

Thm: [Turner, Mukherjee, Boyer 2014]

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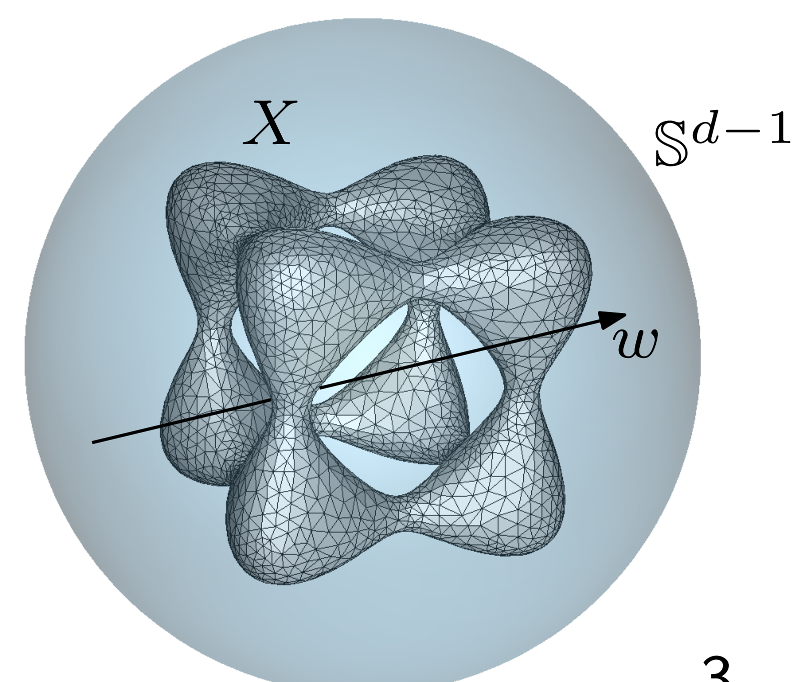
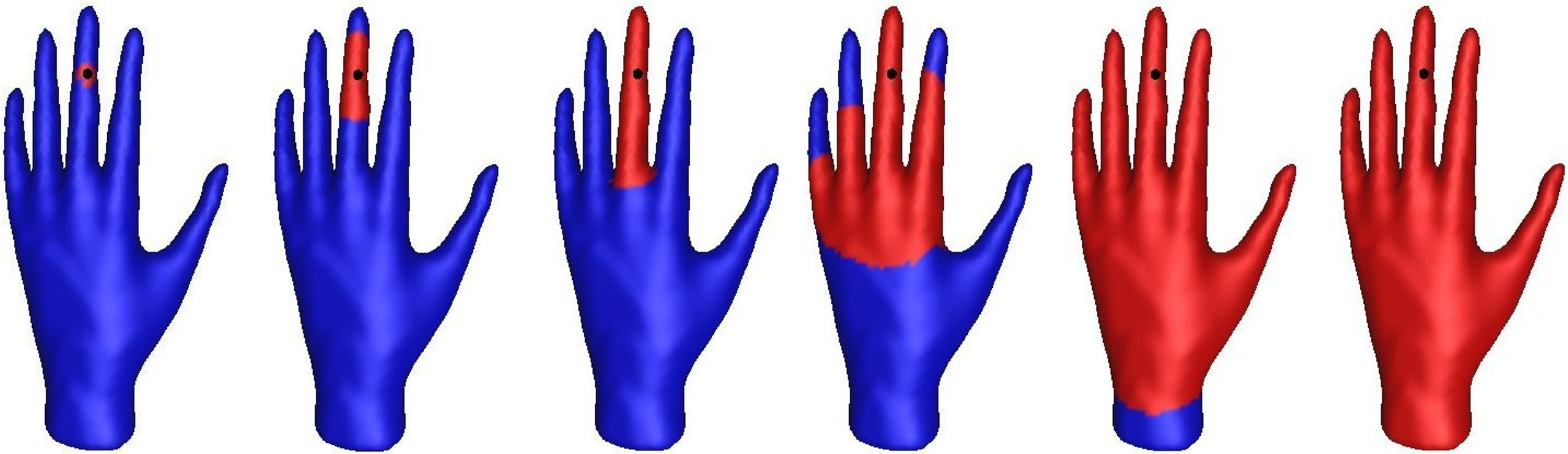


PHT for intrinsic metrics

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



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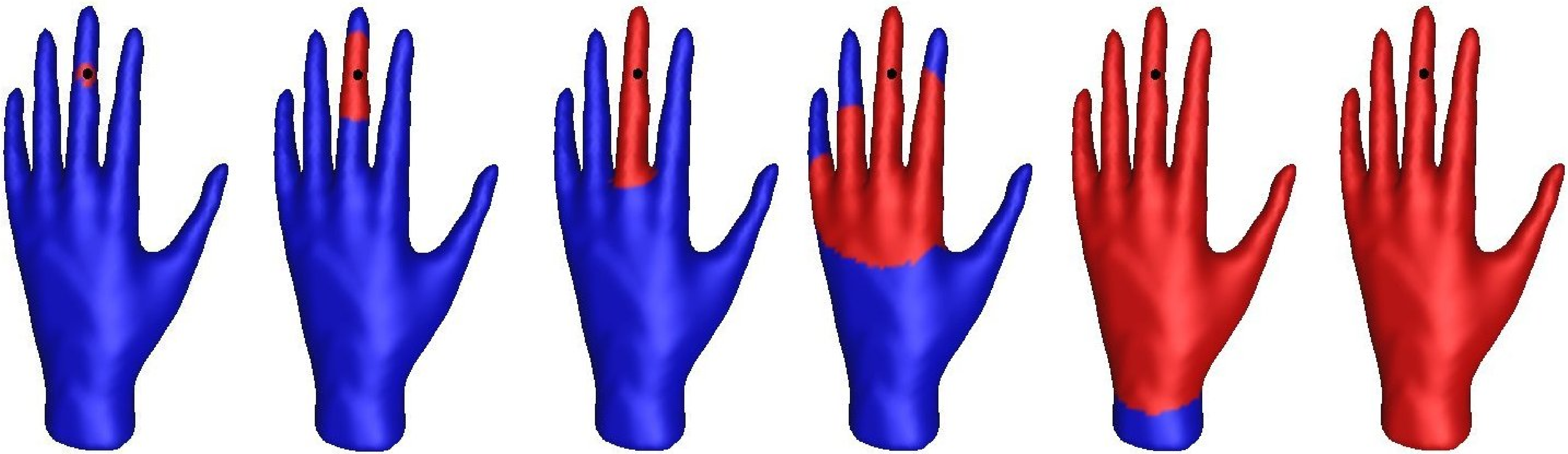

Thm (local stability): [Carrière, O., Ovsjanikov 2015]
Let (X, d_X) and (Y, d_Y) be compact length spaces with positive convexity radius ($\varrho(X), \varrho(Y) > 0$). Let $x \in X$ and $y \in Y$. If $\mathrm{d}_{\mathrm{GH}}((X,x),(Y,y)) \leq \frac{1}{20} \min\{\varrho(X),\ \varrho(Y)\}$, then

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

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

Corollary (local stability of PHT):

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

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

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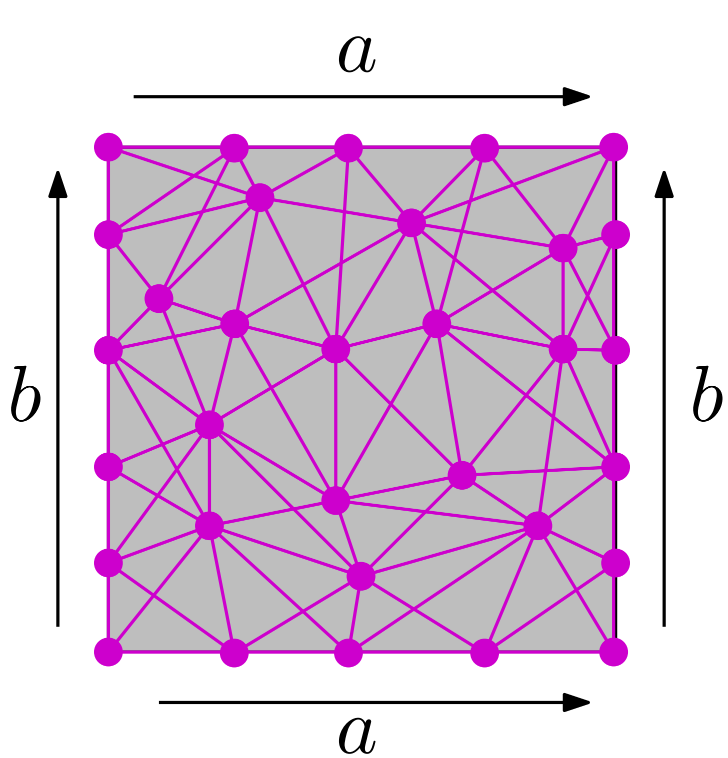

$\mathrm{d}_{\mathrm{GH}}(T, X) \xrightarrow{\#X \to \infty} 0$

$\mathrm{d}_{\mathrm{H}}(\mathsf{PHT}(T), \mathsf{PHT}(X))$ 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.

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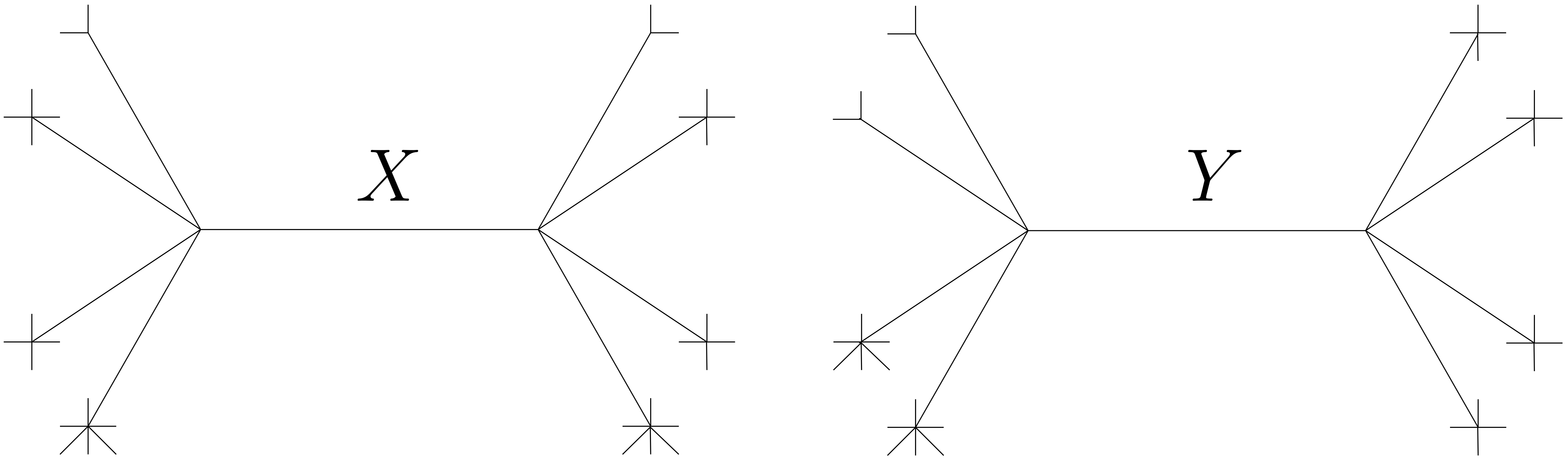
Q: injectivity of PHT on metric graphs?

PHT for metric graphs

Negative result: PHT is not injective on all compact metric graphs



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PHT for metric graphs

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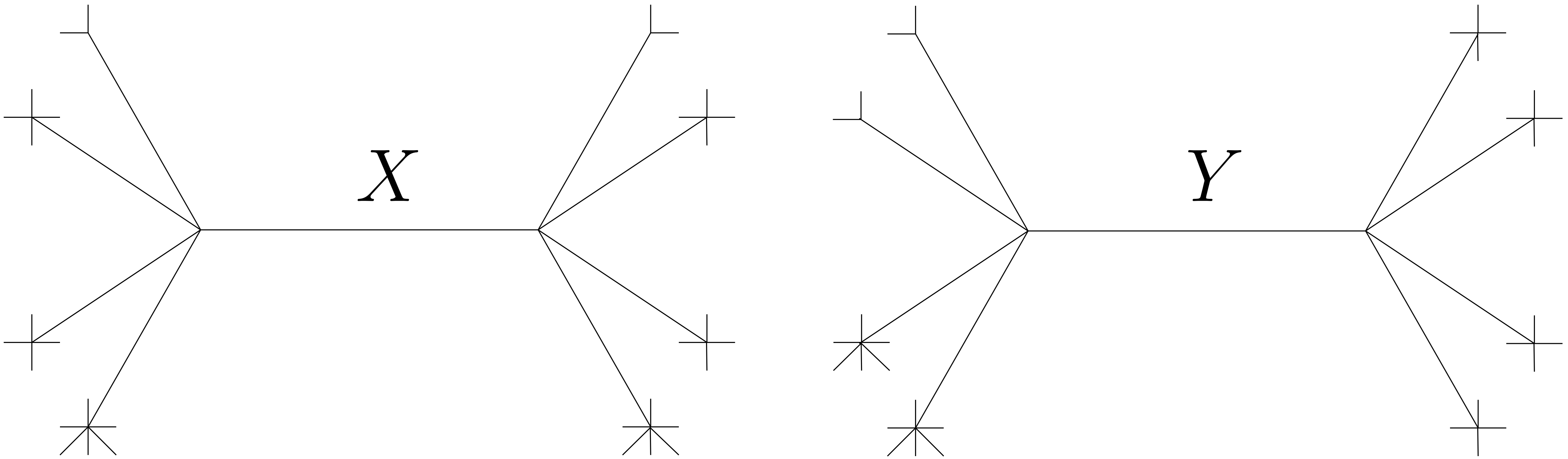


$$\mathsf{PHT}(X) = \mathsf{PHT}(Y) \text{ while } X \not\simeq Y$$

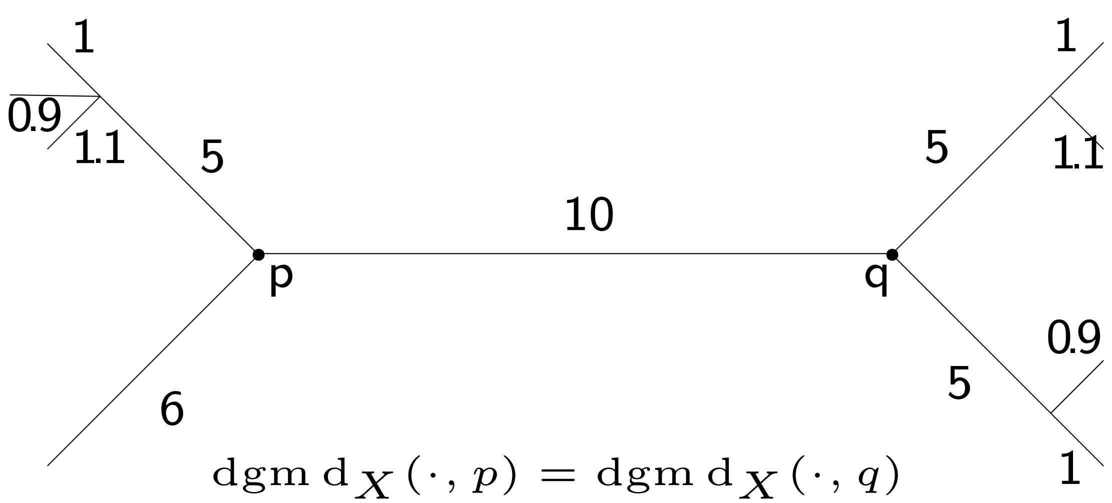
Note: $\mathrm{Aut}(X)$ is non-trivial, hence $\Psi_X : x \mapsto \mathrm{dgm}\,\mathrm{d}_X(\cdot, x)$ is not injective

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 $\underset{\not\Leftarrow}{\Rightarrow}$ Aut(X) trivial

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

+ Gromov's density result

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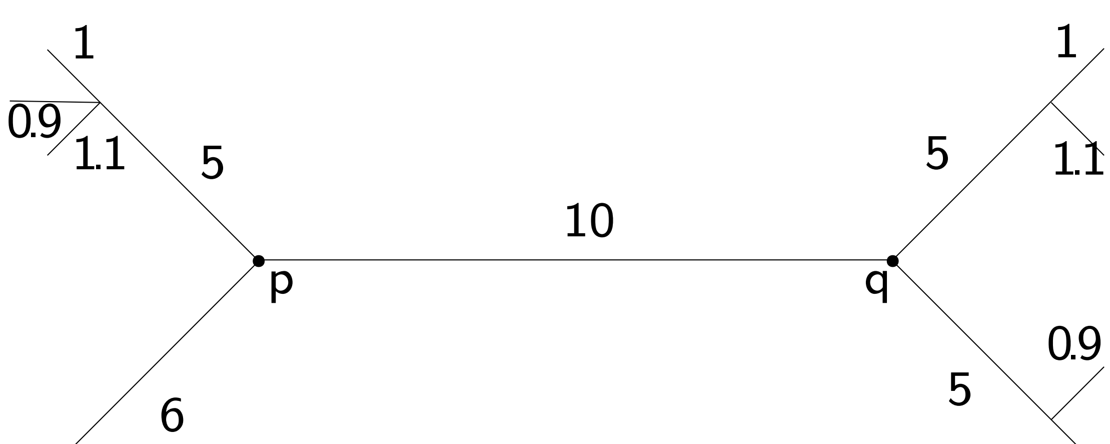
Corollary:

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



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

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PHT for metric graphs

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Thm 3:

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

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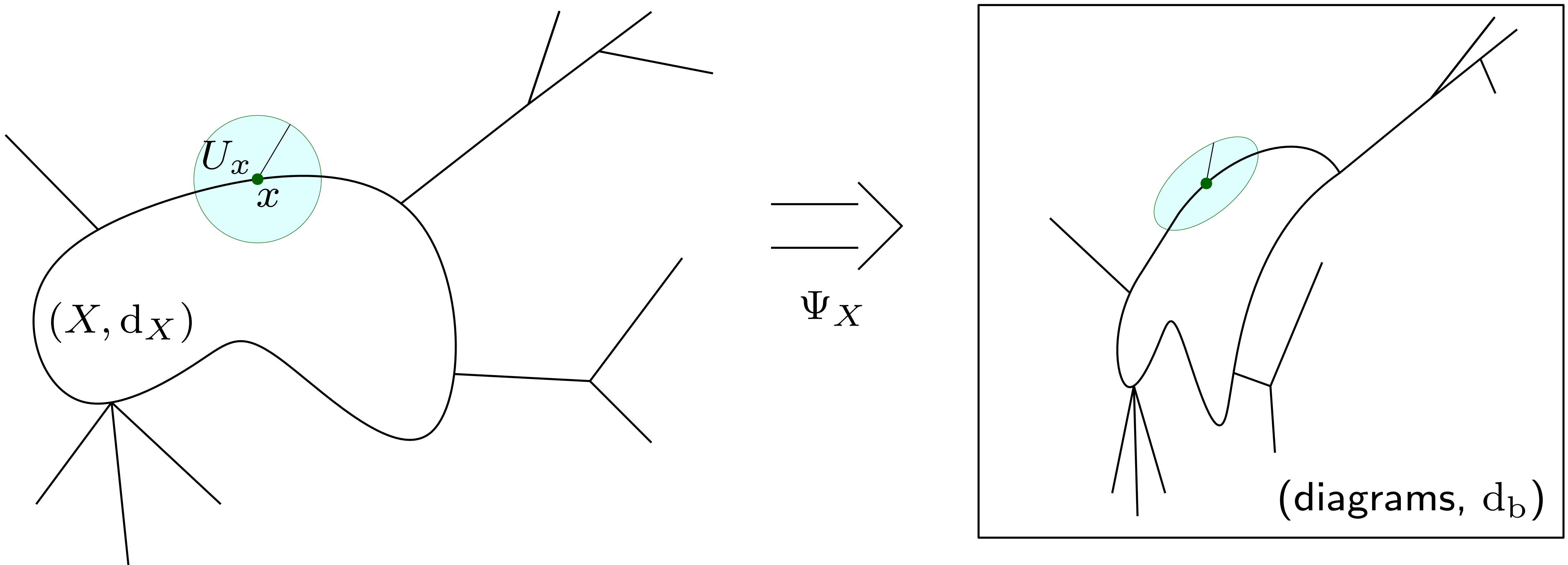
Proof outline for Thm 1

Prop:

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

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



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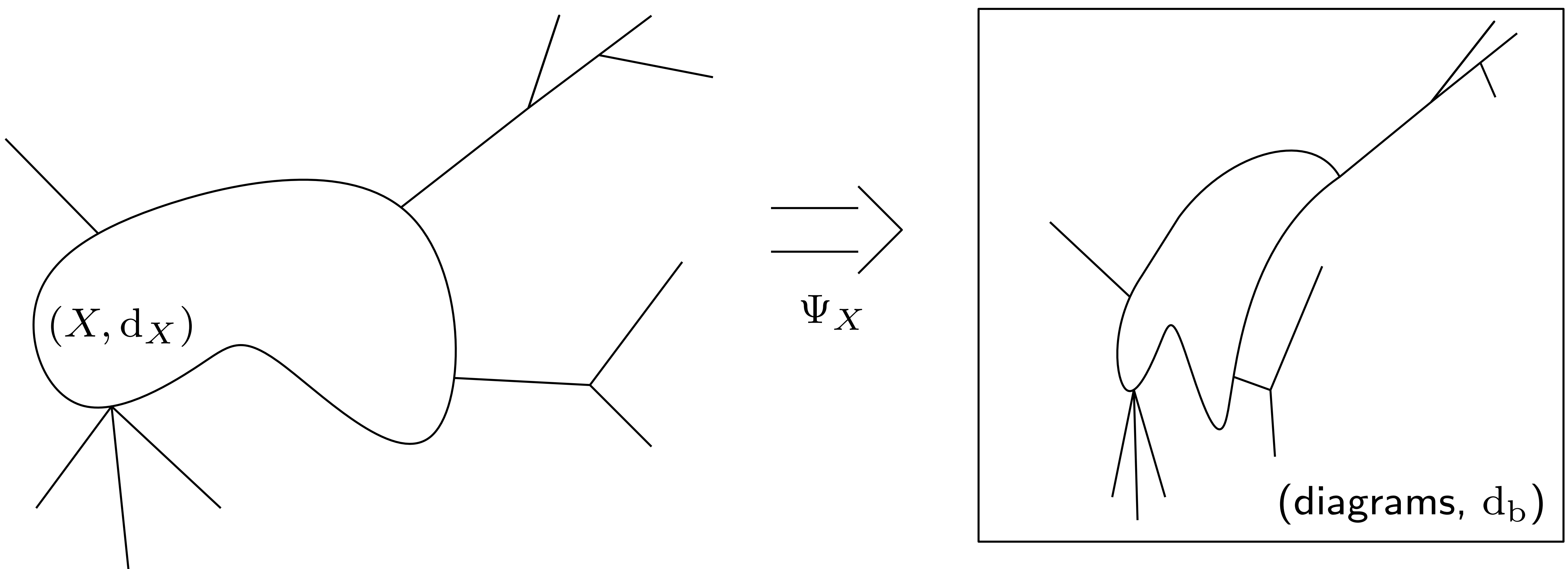
Corollary:

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



Proof outline for Thm 2

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.

Thm 3:

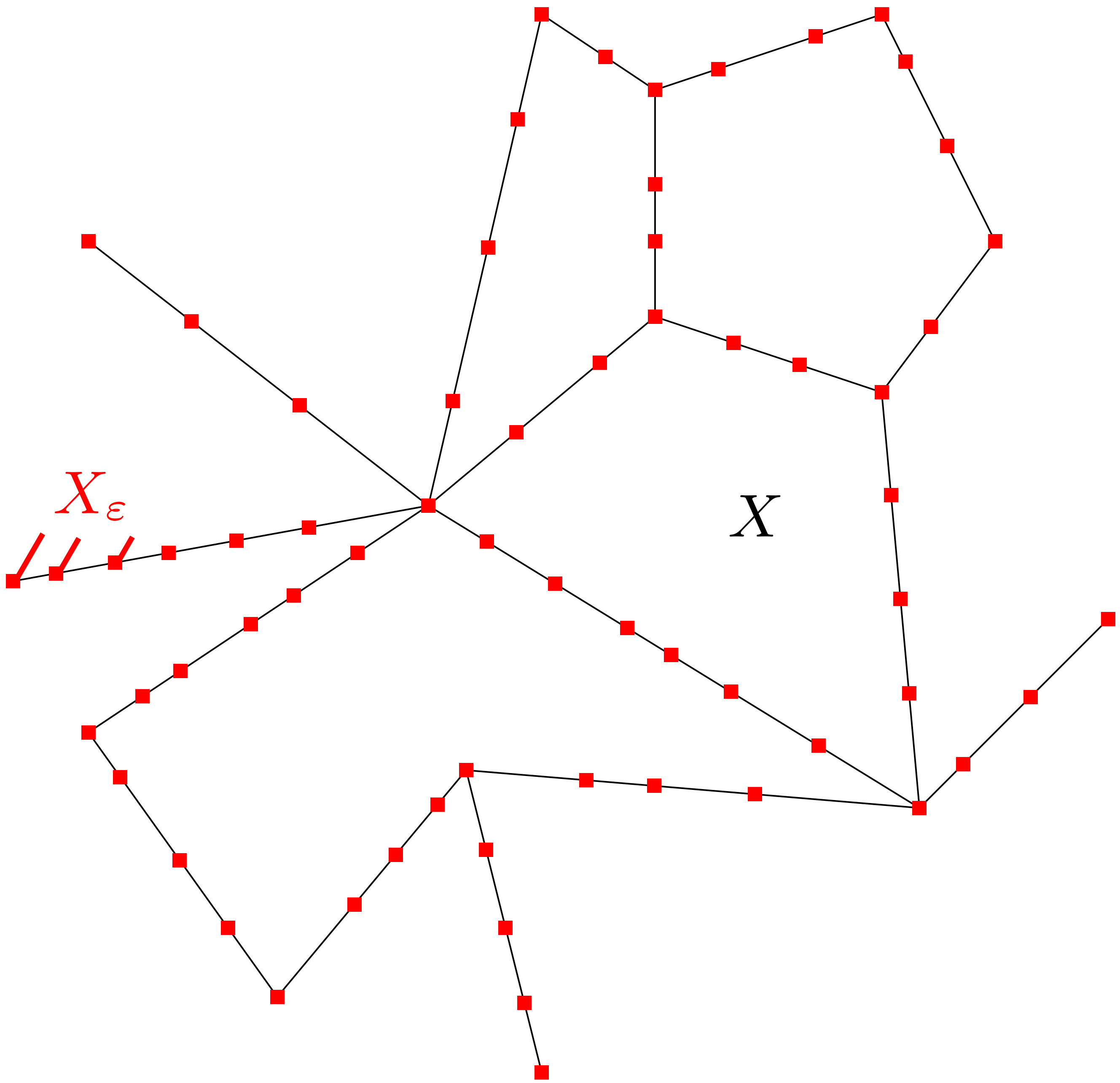
PHT is GH-*locally* injective on compact metric graphs.

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



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Break symmetries by *cactification*:

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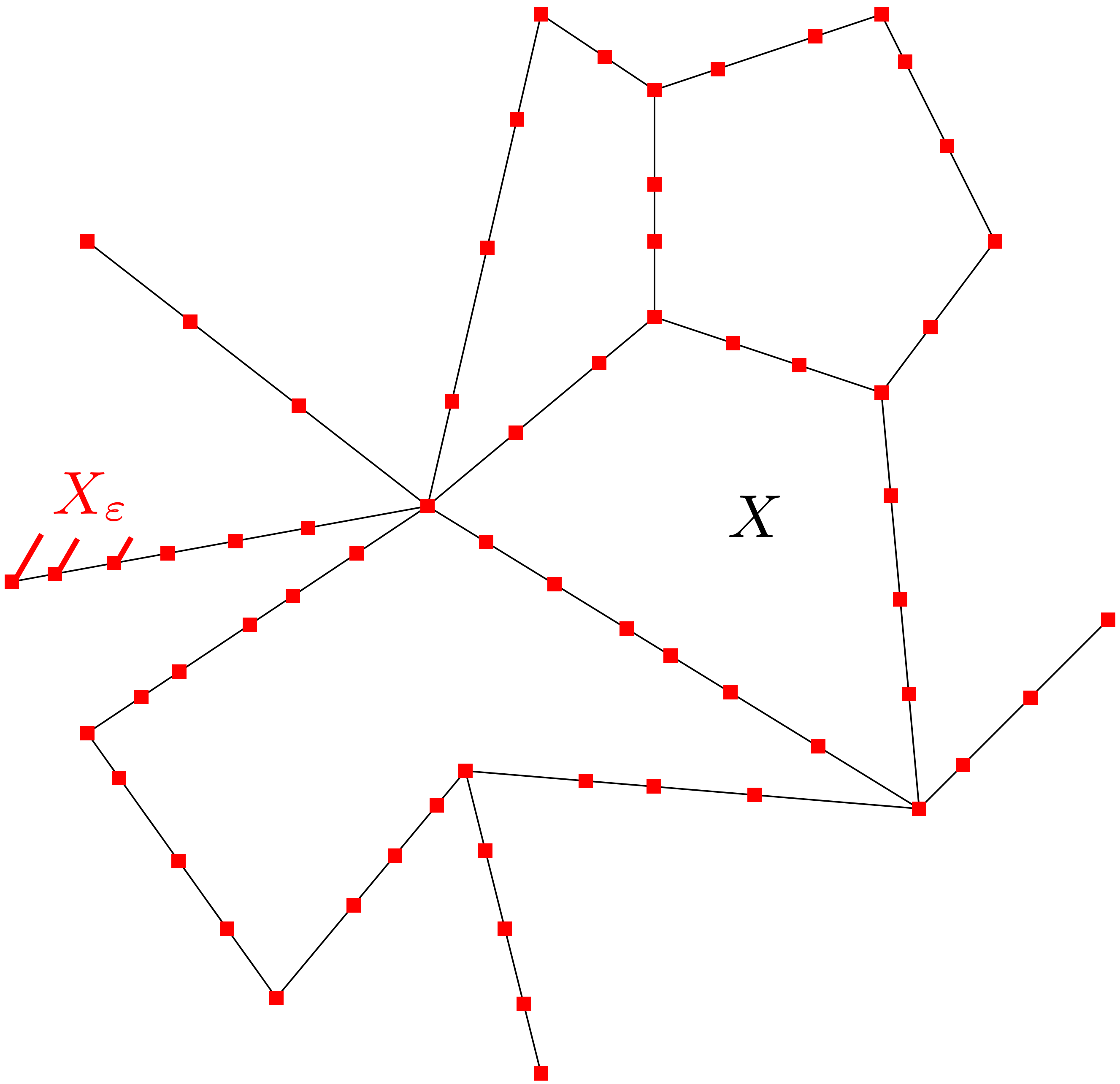
$\rightarrow$ $(X_\varepsilon, \mathrm{d}_{X_\varepsilon})$ parametrized by distances to thorn bases and tips

$\rightarrow$ these distances appear in the persistence diagrams



Proof outline for Thm 3

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

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Thm 1:

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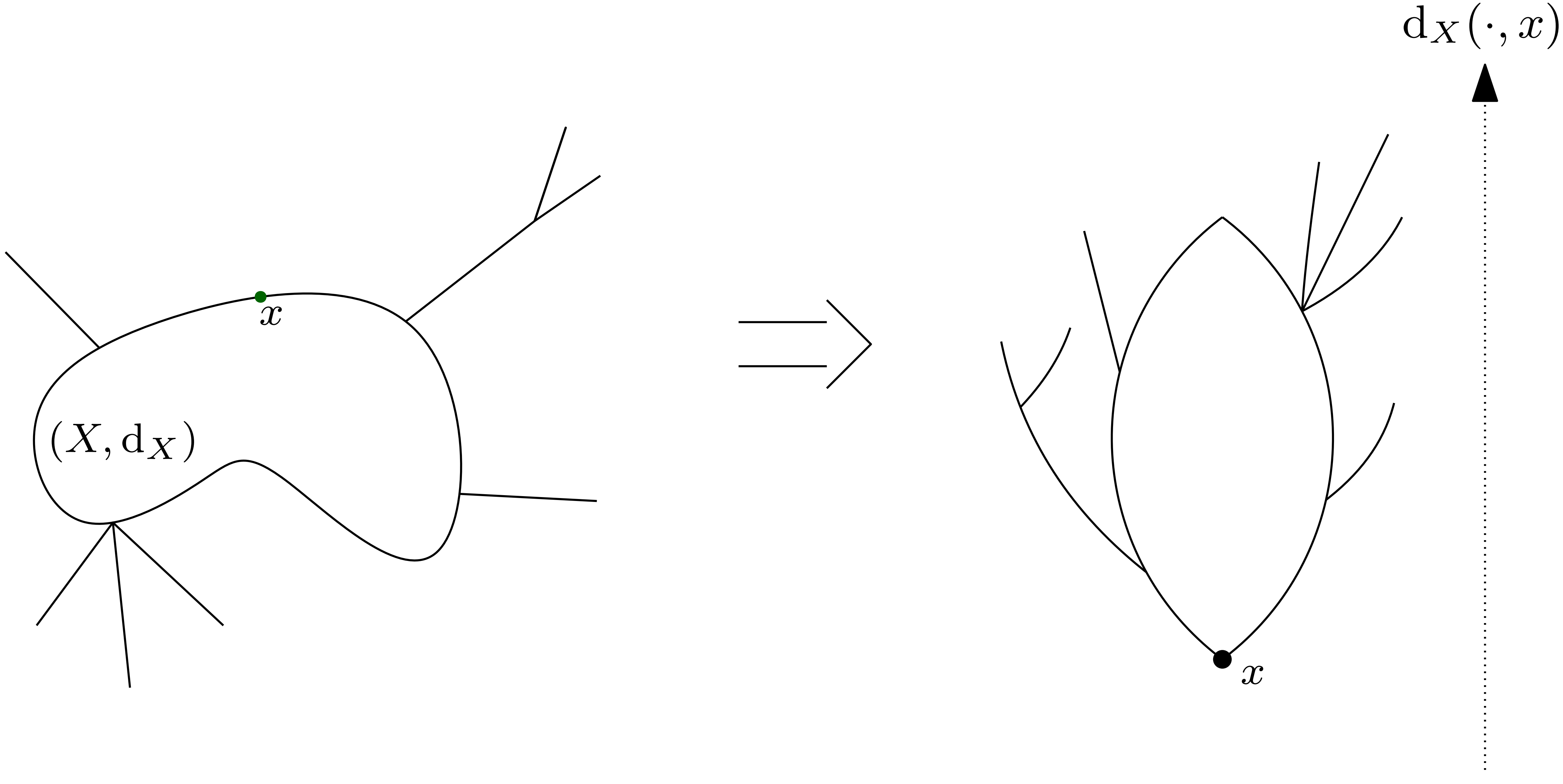
Proof outline for Thm 3

Prop:

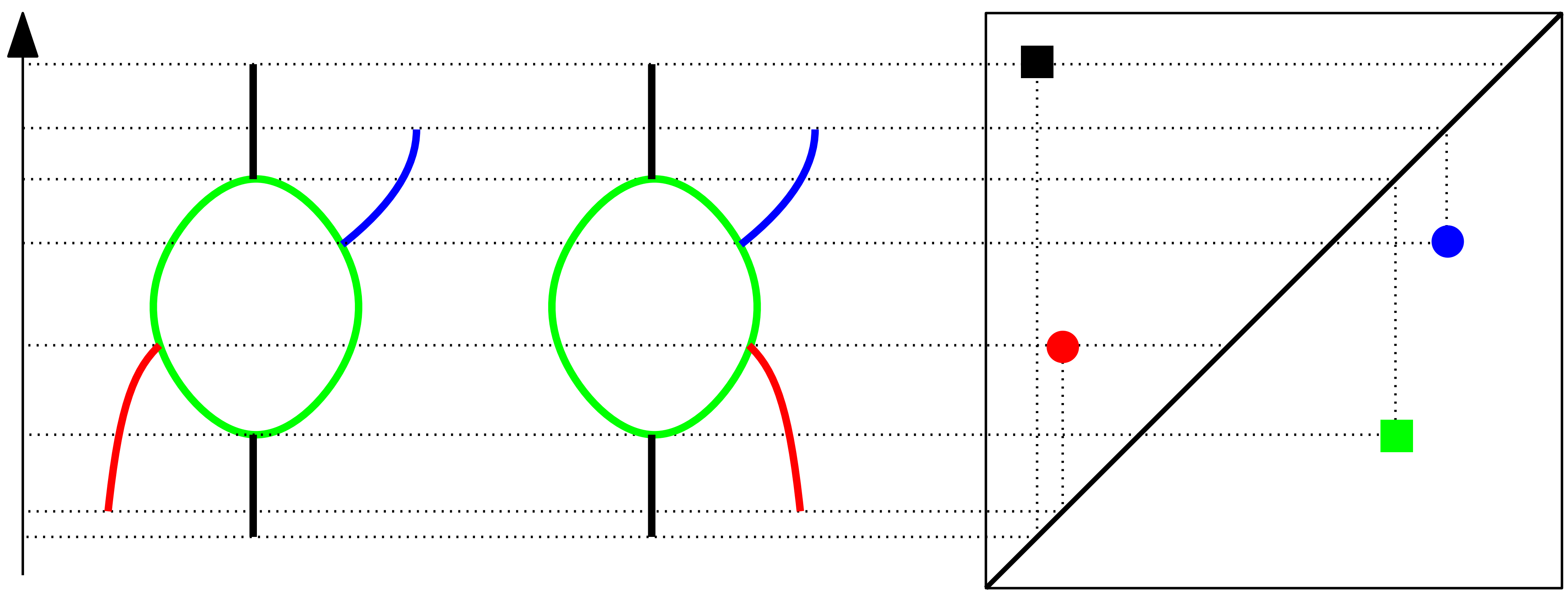
The map $(X, \mathrm{d}_X, x) \mapsto R_{\mathrm{d}_X(\cdot,x)}$ is injective.



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.

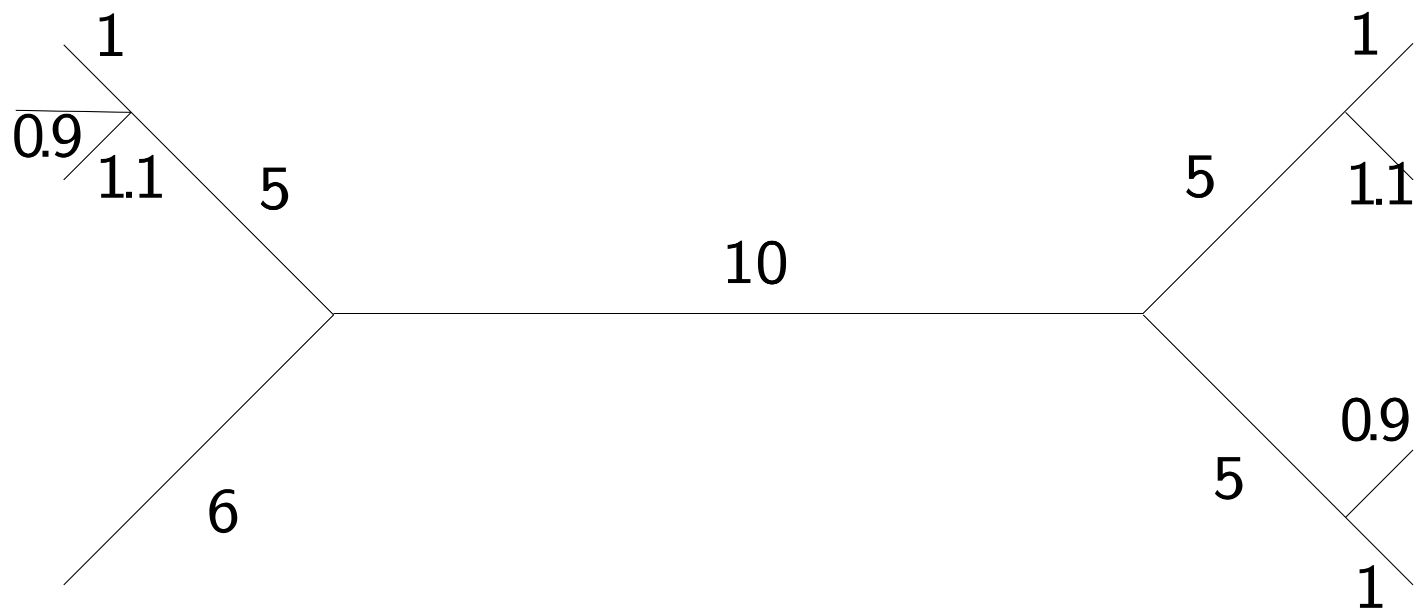


Generic injectivity

Generative model:

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

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



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

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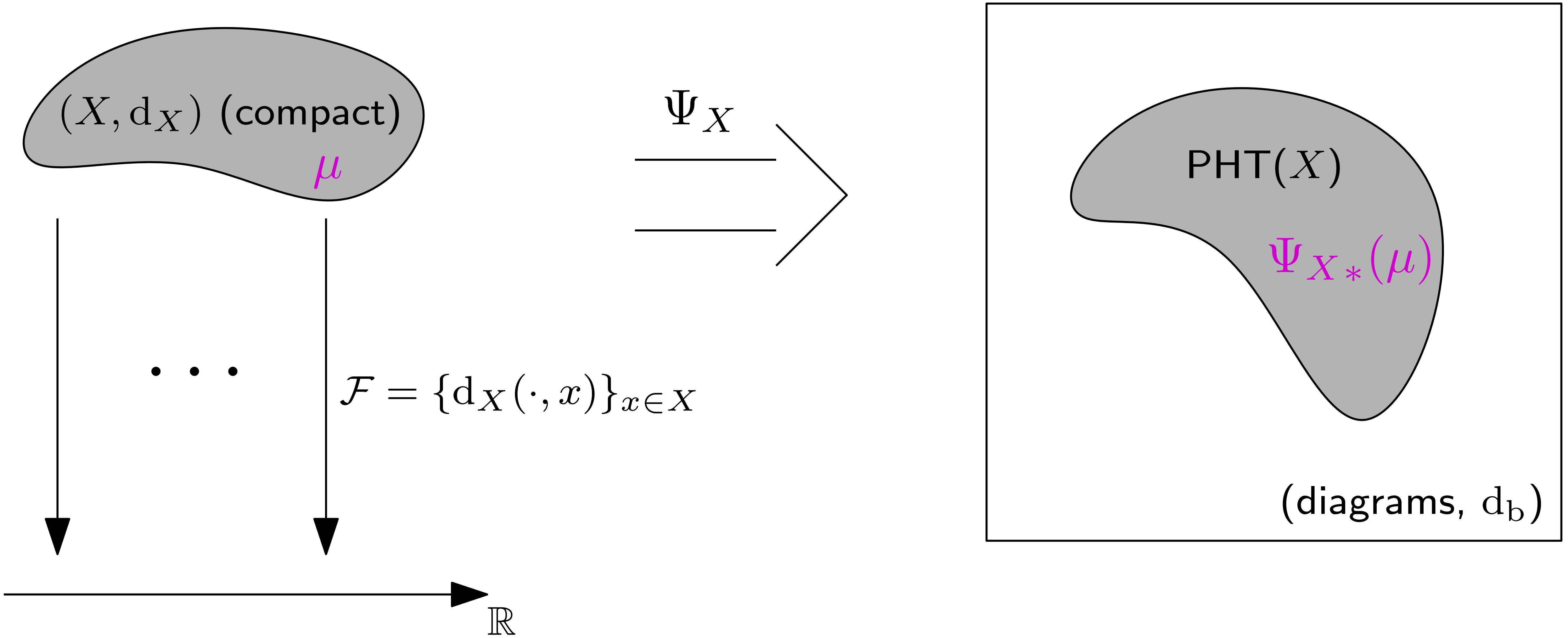
Thm 4:
Under this model, there is a full-measure subset of the metric graphs on which PHT is injective.

Proof outline:

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

Measure-theoretic view



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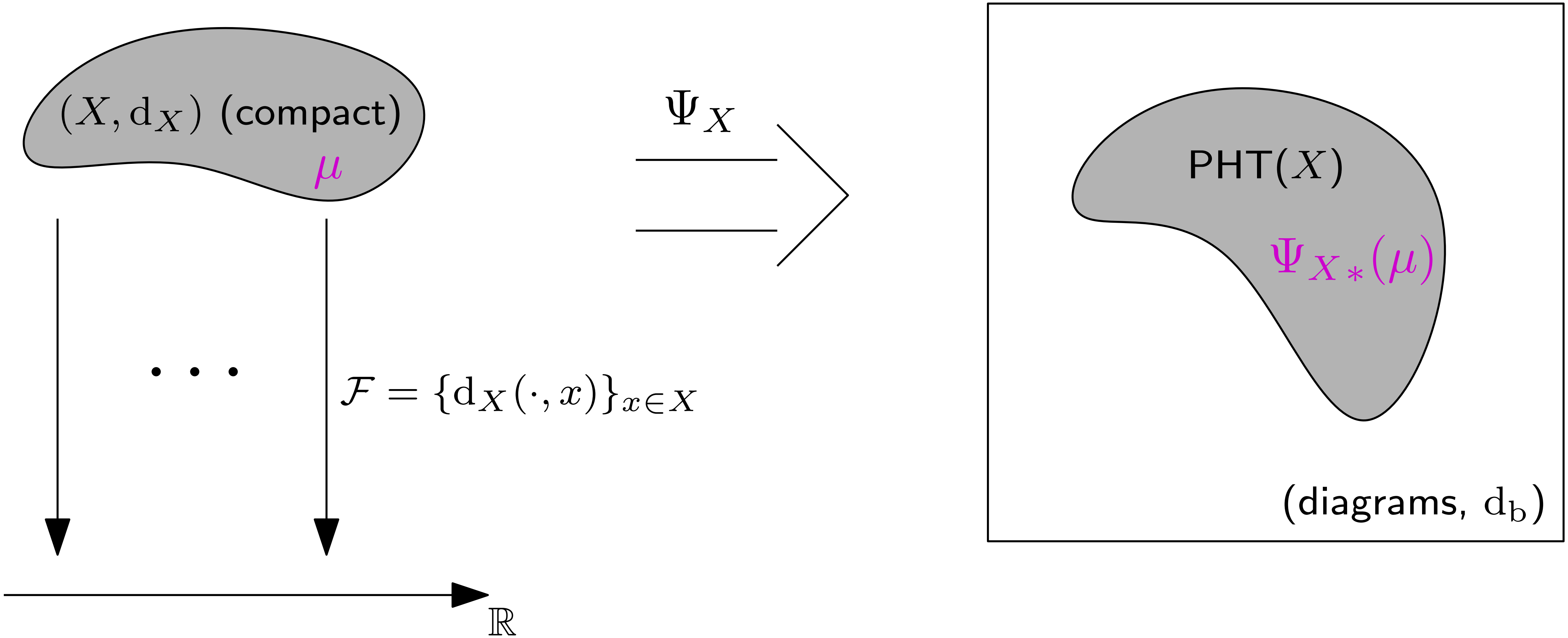
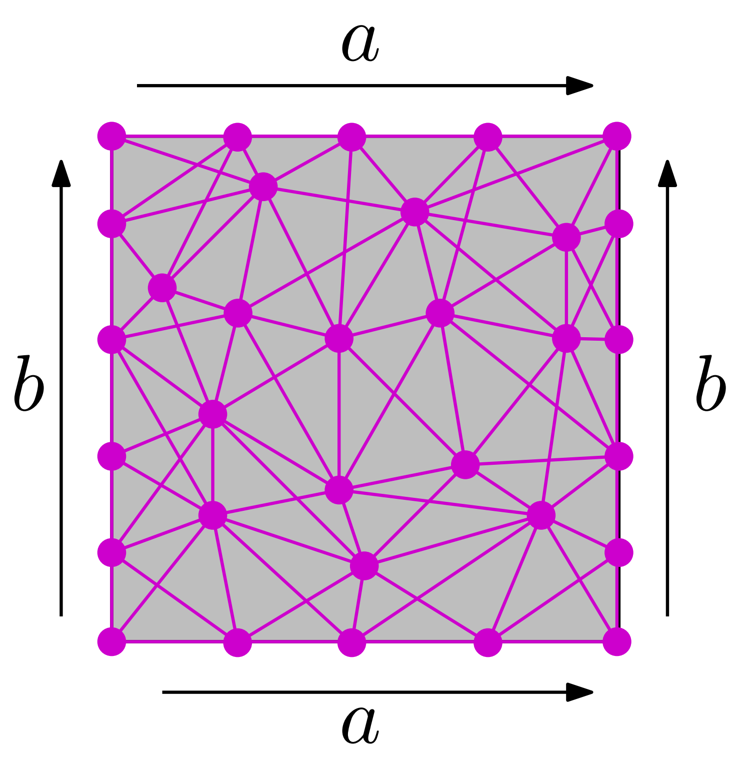


Thm 5 (remark):
$(X, \mu) \mapsto (\mathsf{PHT}(X), \Psi_{X*})$ is injective on those measure metric graphs (X, μ) such that $X \in \mathsf{Inj}_\Psi$.

Perspectives

Higher-dimensional length spaces

- limit argument



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

$\mathrm{d_H}(\mathsf{PHT}(T), \mathsf{PHT}(X))$ is bounded away from 0

Pb: GH-convergence $\not\Rightarrow$ $\mathrm{d_b}$-convergence

- spectral embedding $+$ extrinsic framework