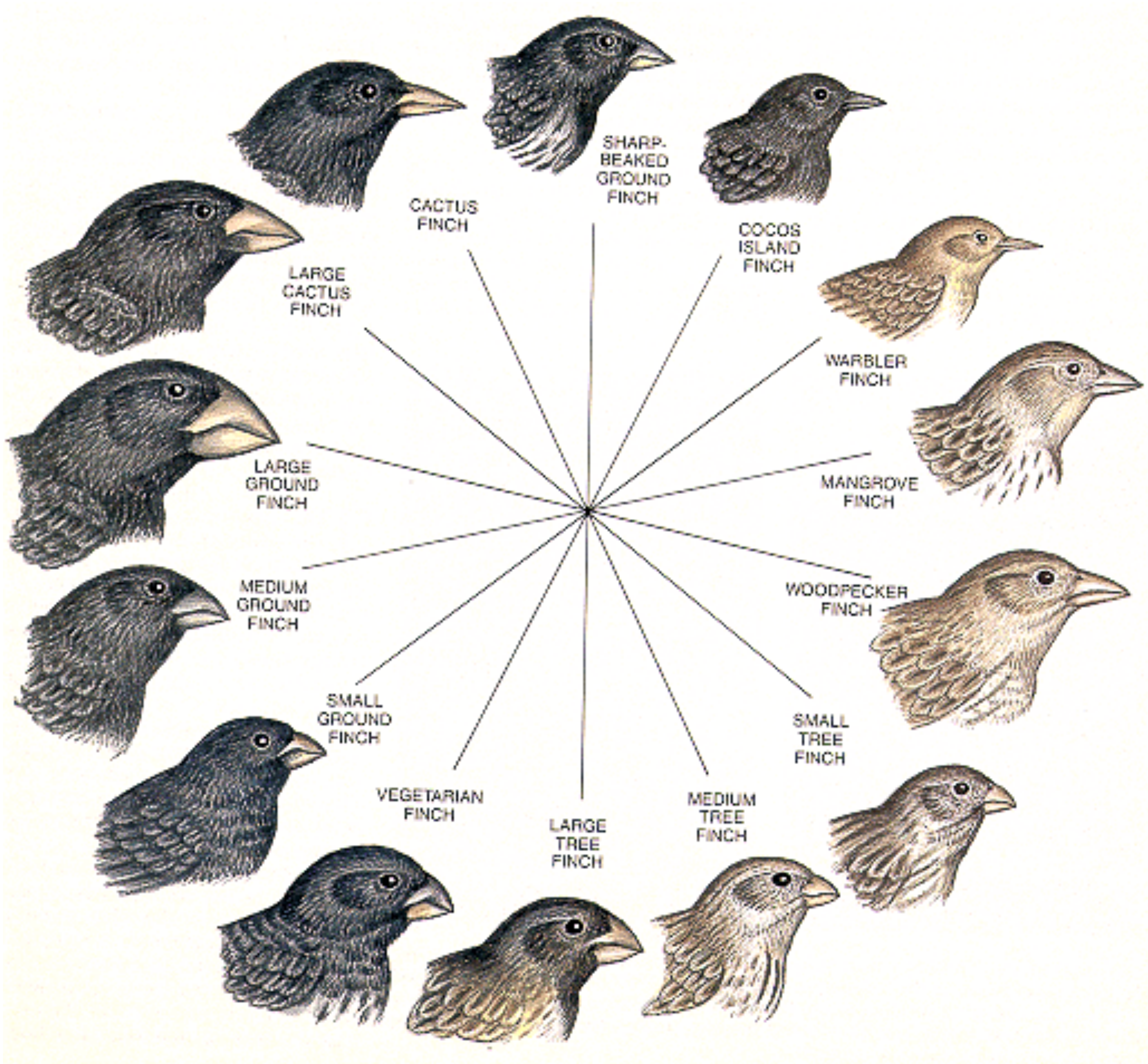
How Many Directions Determine a Shape

Sayan Mukherjee, Duke University

Robust and High-Dimensional Statistics
Berkeley, CA
https://sayanmuk.github.io/

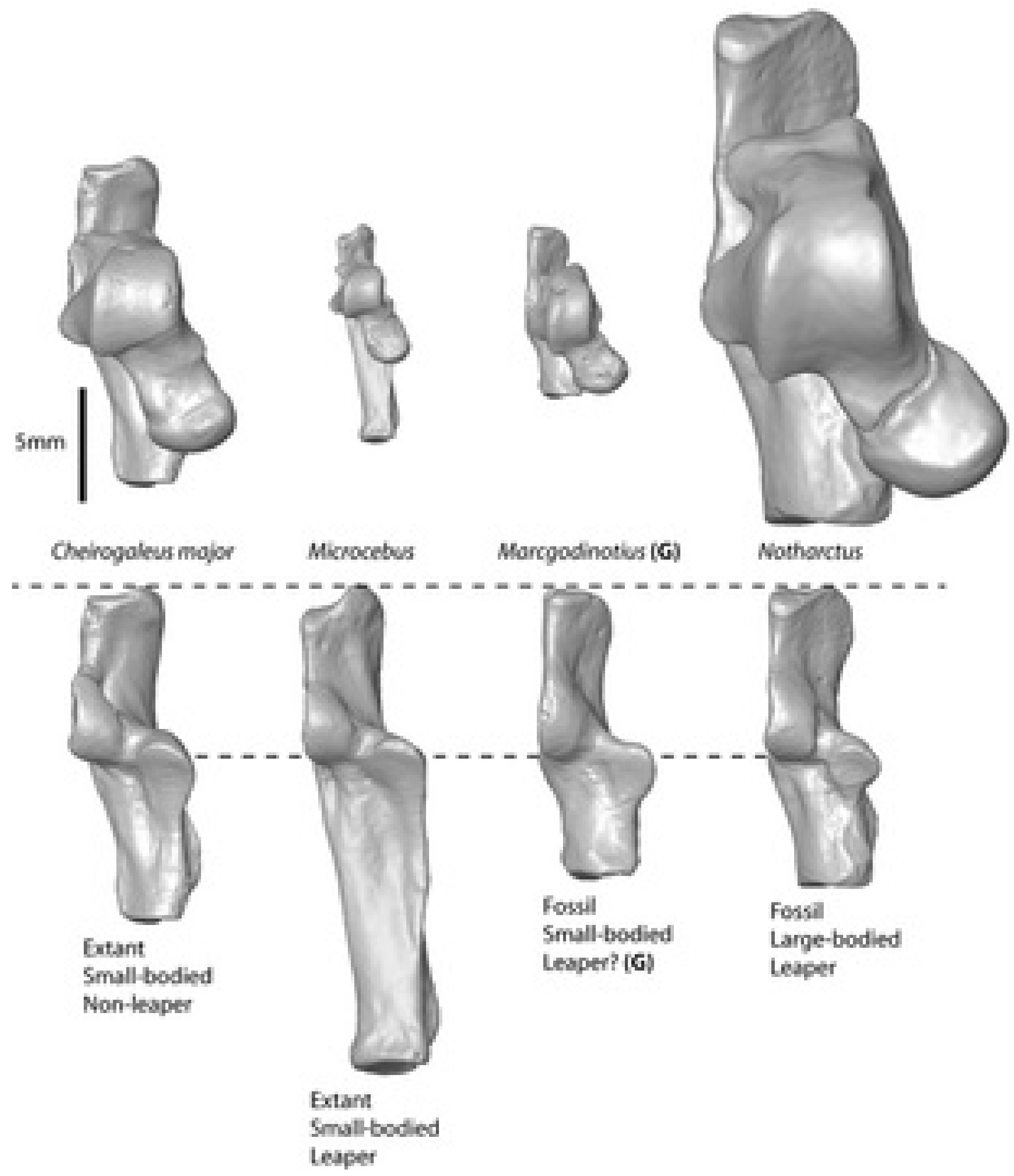
Digital phenotyping — J. Curry, K. Turner, D. Boyer
— L. Crawford, A. Monod, R. Rabadán, A. Chen

Modeling variation in shapes



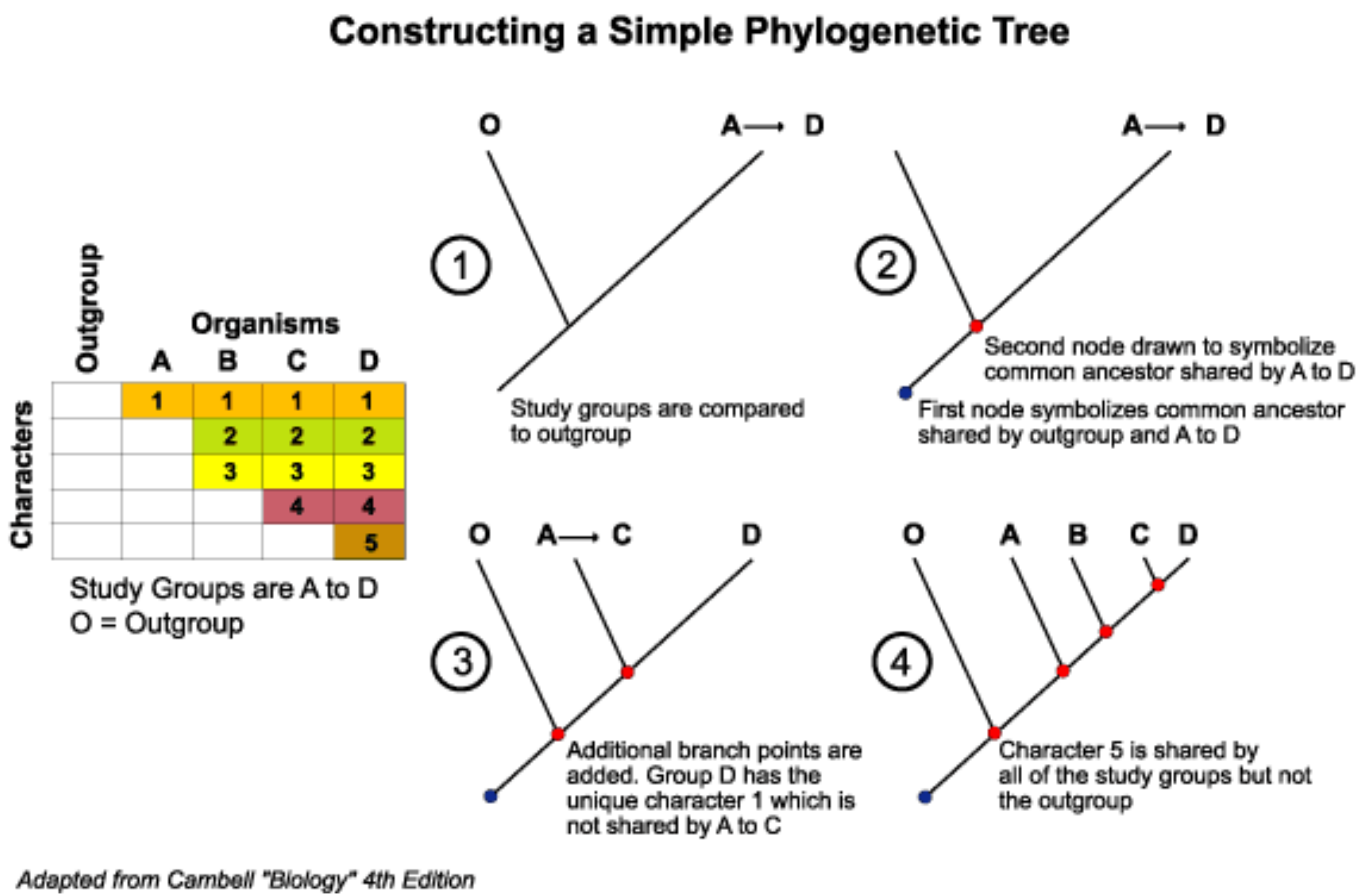
S. J. Gould

Variation in calcanei



D. Boyer.

From distances to trees



Evolution as broccoli

Models of surfaces

(1) Shape spaces: Kendall, D. G. (1984) Shape manifolds, procrustean metrics, and complex projective spaces. Bull. Lond. Math. Soc., 16, 81121.

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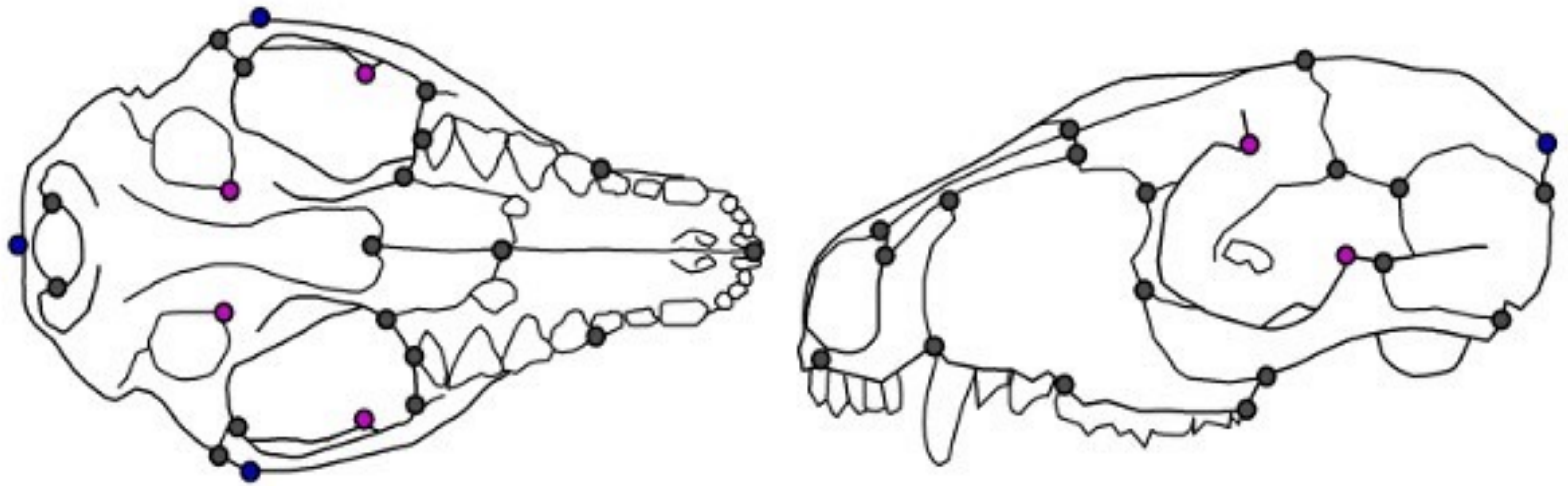
(3) Integral geometry: Worsley, K. J. (1995) Estimating the number of peaks in a random field using the Hadwiger characteristic of excursion sets, with applications to medical images. Ann.Stat., 23, 640669.

Landmarks and shape spaces



Procrustes distance and shape space

For an object i: L landmarks $(o_{\ell,i})_{\ell=1}^{L}$ with each $o_{\ell,i} \in \mathbb{R}^d$.

The procrustes distance between two points is

$$d_p(o_i, o_j) = \min_{T \in \mathcal{T}} \frac{1}{L} \sum_{\ell=1}^{L} (o_{\ell,i} - T o_{\ell,j})^2,$$

$\mathcal{T}$ are rotations, translations, and scalings.

Kendall's shape space: $M_{d,\ell}$ are $d \times \ell$ matrices

$$F_d^\ell := M_{d,\ell} \setminus \{0\}, \quad S_d^\ell := \{x \in F_d^\ell : \|x\| = 1\}$$

$$\Sigma_d^\ell := S_d^\ell / SO(d) := \Big\{[x] : x \in S_d^\ell \text{ such that } [x] = \{gx : g \in SO(d)\}\Big\}.$$

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foot of Daubentonia madagscariensis *scanned at 38micron resolution at Duke Evolutionary Anthropology department's new high resolution microCt facility. Click here if you are interested in details on the facility*

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Four bones of a new species of Homo from South Africa.

➔ See all the bones of the newly described Homo naledi

➔ Read the published article

PREVIOUS NEXT

Welcome

MorphoSource is a project-based data archive that allows researchers to store and organize, share, and distribute their own 3d data. Furthermore any registered user can immediately search for and download 3d morphological data sets that have been made accessible through the consent of data authors.

The goal of **MorphoSource** is to provide rapid access to as many researchers as possible, large numbers of raw microCt data and surface meshes representing vouchered specimens.

File formats include tiff, dicom, stanford ply, and stl. The website is designed to be self explanatory and to assist you through the process of uploading media and associating it with meta data. If you are interested in using the site for your own data but have questions about security or anything else contact the site administrator. Otherwise please download whatever data you need and check back frequently to see what's new.

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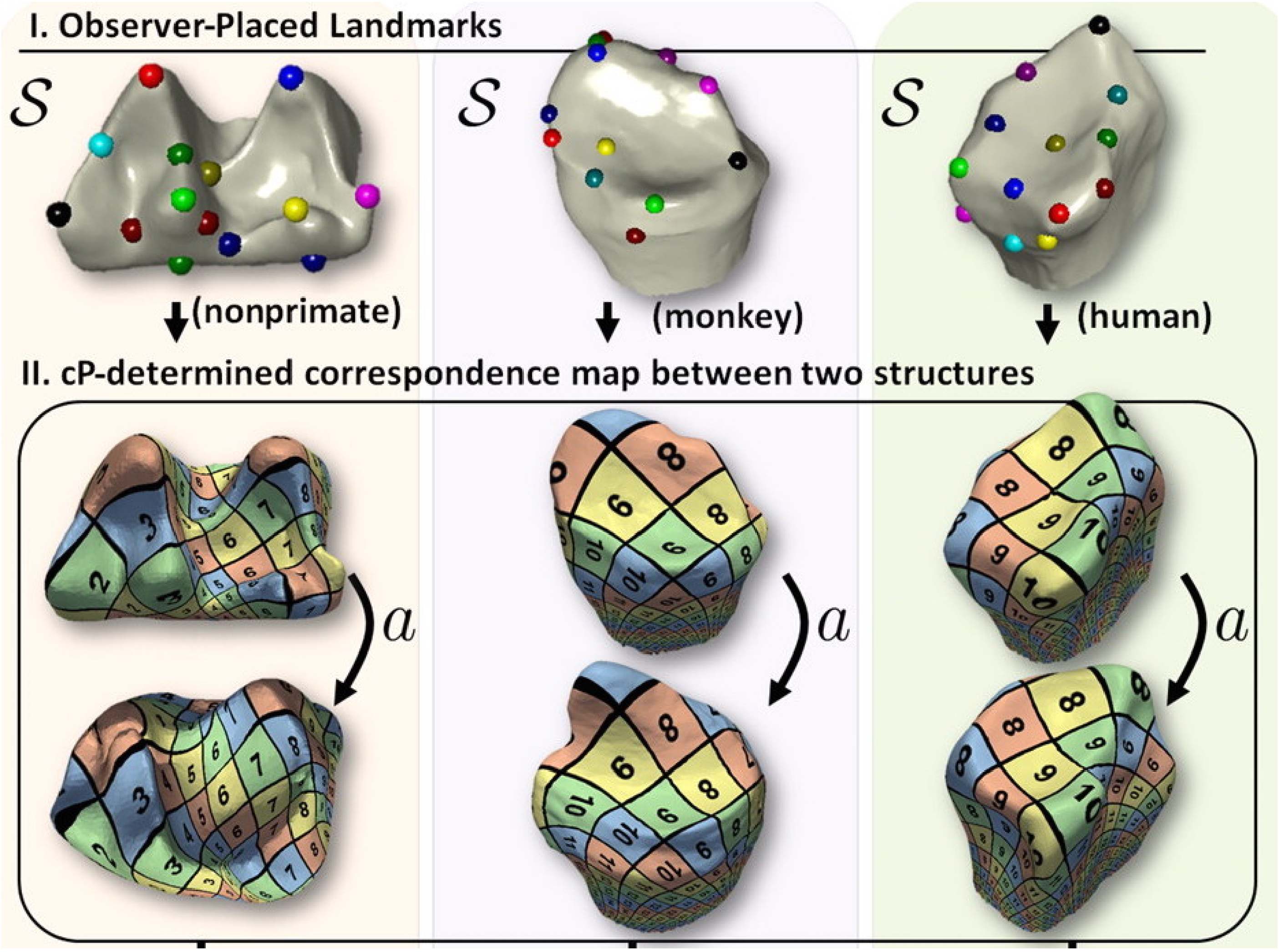
Diffeomorphism based approach

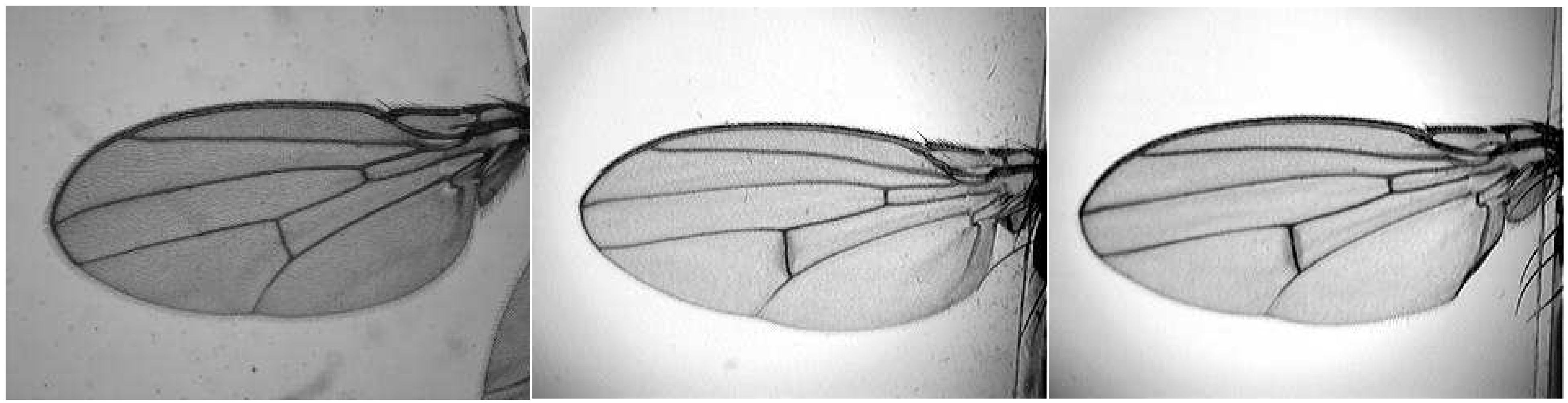
Similarity between teeth: Algorithms to automatically quantify the geometric similarity of anatomical surfaces, Boyer et. al. PNAS 2011.



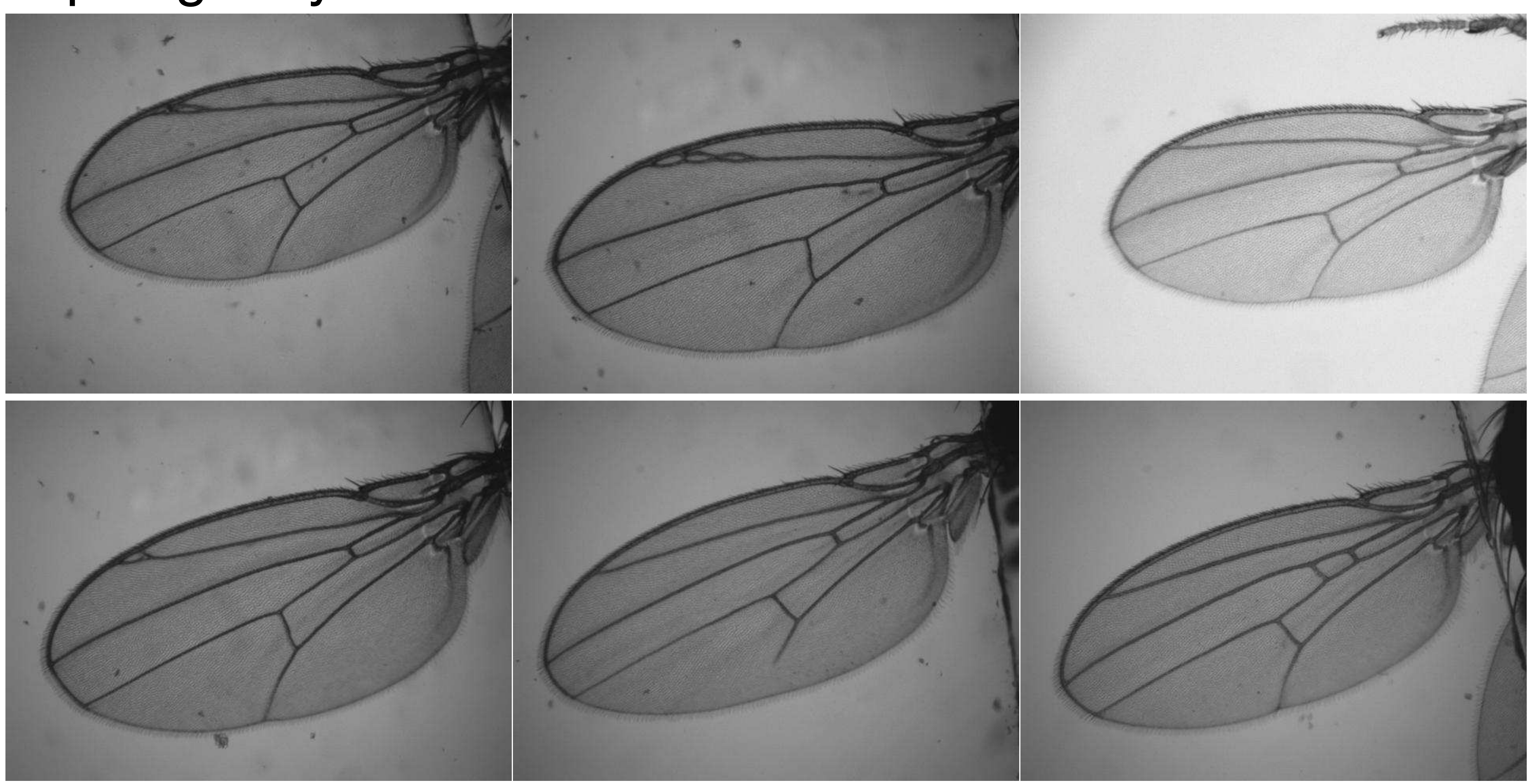
Homeomorphism between shapes

Fly wings are not homeomorphic

Normal fly wings [photos from David Houle's lab]:



Topologically abnormal veins:



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(3) Pull back from the transformed space to positions on shapes.

Two topological summaries

(1) Euler characteristics.

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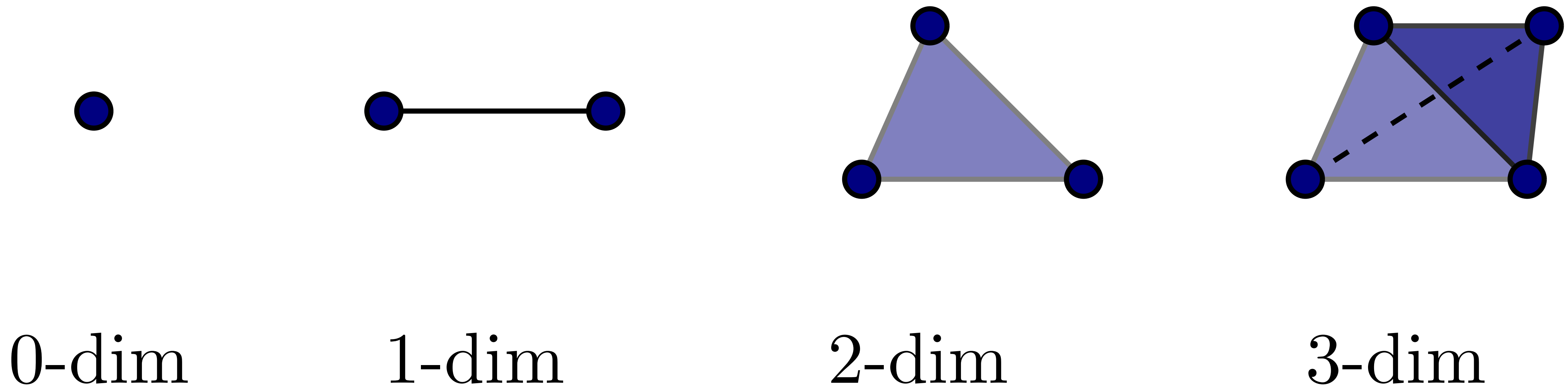
(2) Persistent homology.

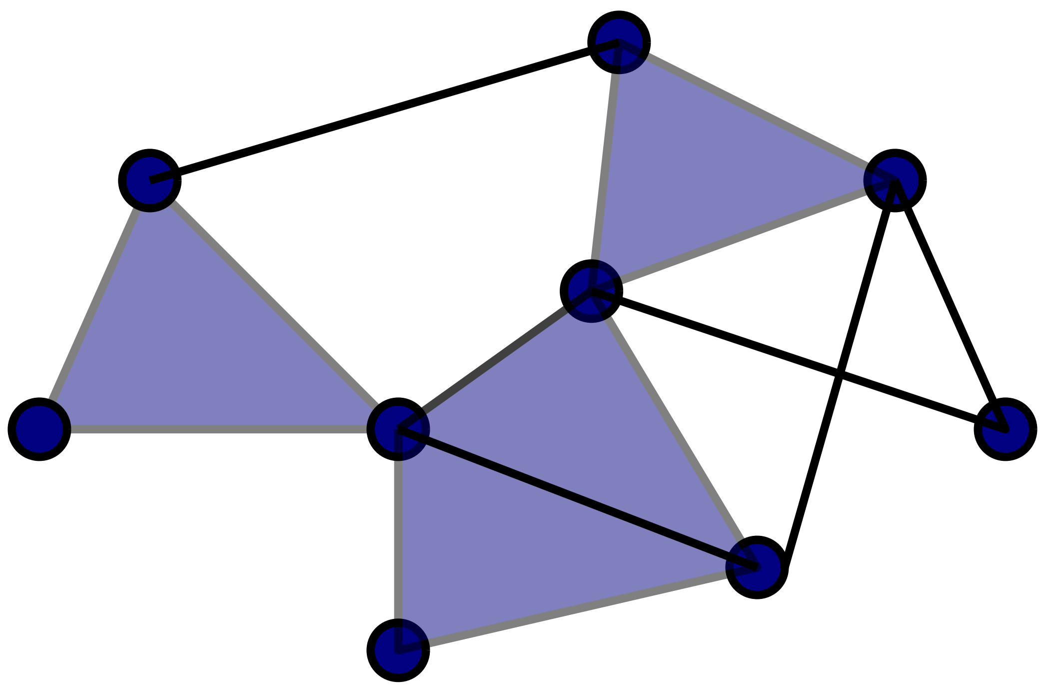
Simplices



Simplicial Complexes

Collection of simplices glued together in a special way

- All faces of a simplex are in the complex
- Simplices intersect along common faces



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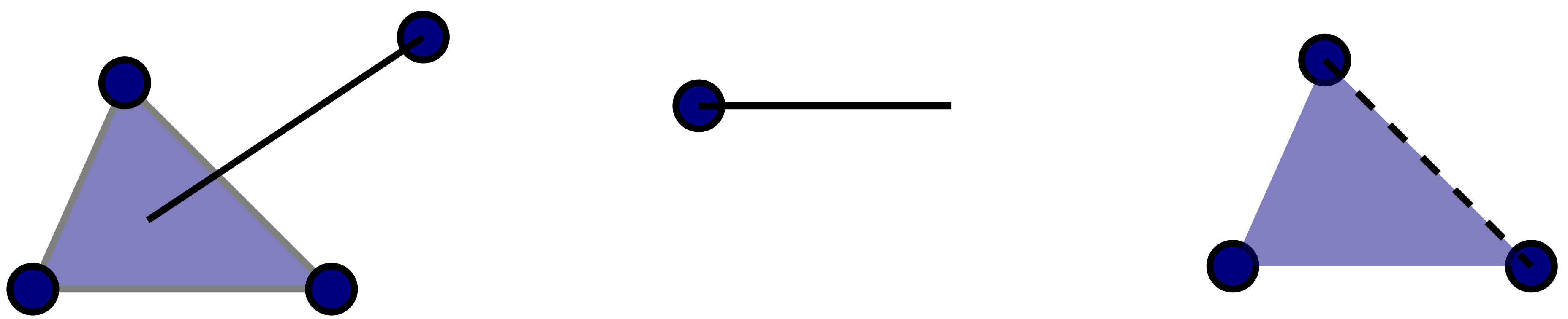

Mathematically what is a shape: less abstract

Definition

A finite geometric simplicial complex K is a finite set of geometric simplices such that

(1) *Every face of a simplex in K is also in K;*

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(1) *Every face of a simplex in K is also in K;*

(2) *If two simplices σ_1, σ_2 are in K then their intersection is either empty or a face of both σ_1 and σ_2.*

Mathematically what is a shape: more abstract

Definition

An o-minimal structure $\mathcal{O} = \{\mathcal{O}_d\}$ specifies for each $d \geq 0$, a collection of subsets $\mathcal{O}_d$ of $\mathbb{R}^d$ closed under intersection and complement. These collections are related to each other by the following rules:

1. *If $A \in \mathcal{O}_d$, then $A \times \mathbb{R}$ and $\mathbb{R} \times A$ are both in $\mathcal{O}_{d+1}$; and*
2. *If $A \in \mathcal{O}_{d+1}$, then $\pi(A) \in \mathcal{O}_d$ where $\pi : \mathbb{R}^{d+1} \to \mathbb{R}^d$ is axis-aligned projection.*

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We further require that $\mathcal{O}$ *contains all algebraic sets and that* $\mathcal{O}_1$ *contain no more and no less than all finite unions of points and open intervals in* $\mathbb{R}$*.*

Constructible sets and functions

Constructible sets $\mathrm{CS}(\mathbb{R}^d)$ are the collection of compact definable subsets of $\mathbb{R}^d$, elements of $\mathcal{O}$.

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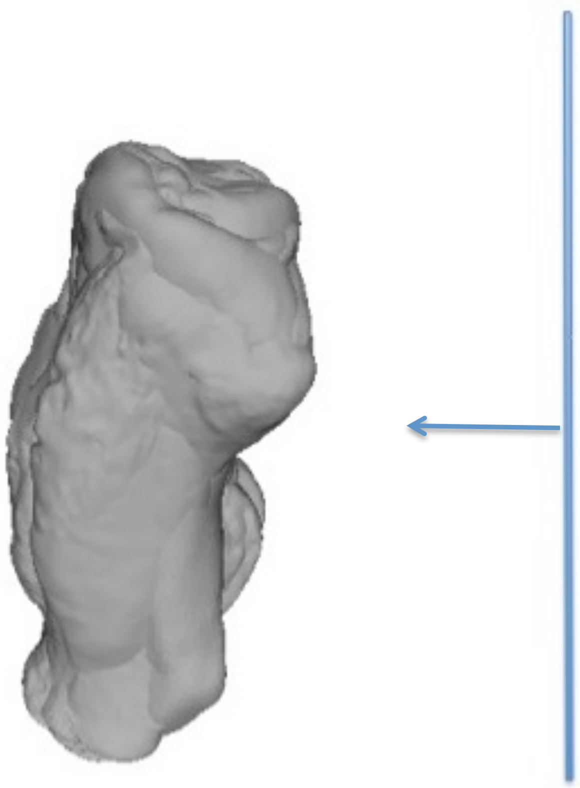
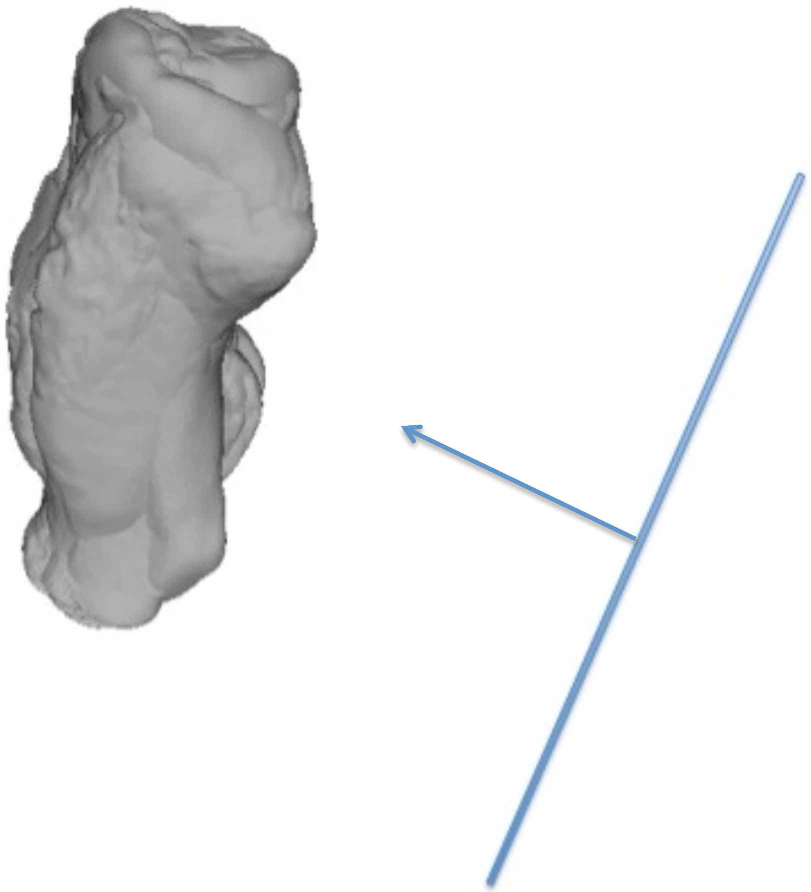
A constructible function is an integer-valued function on a tame set X with the property that every level set is tame.
We denote $\mathrm{CF}(X)$ as the set of constructible functions with domain X.

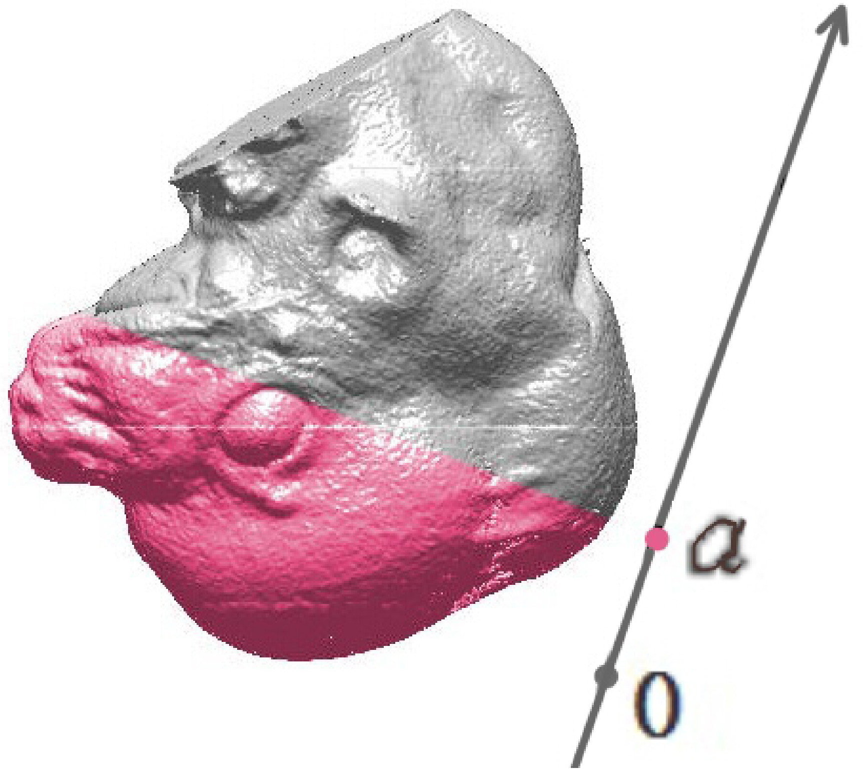
Height function: v_1



Height function: v_2



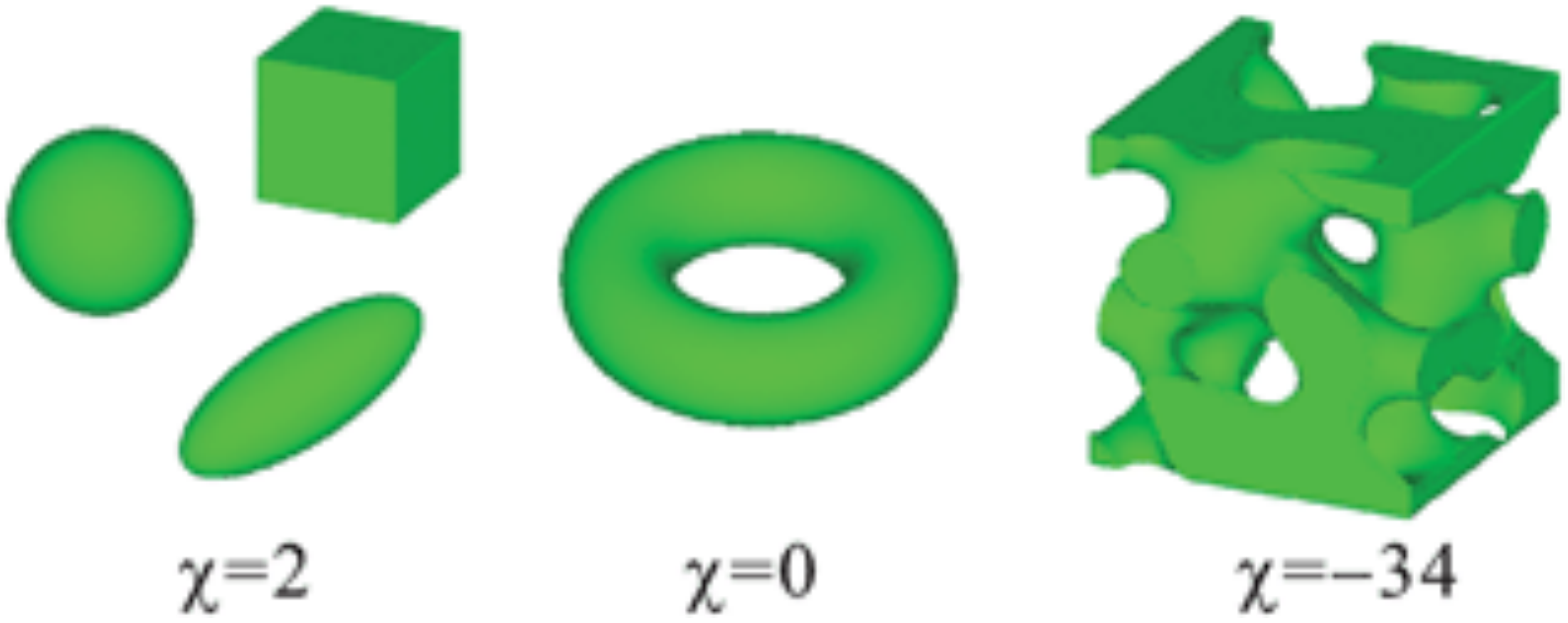
Sublevel set of mouse embryo



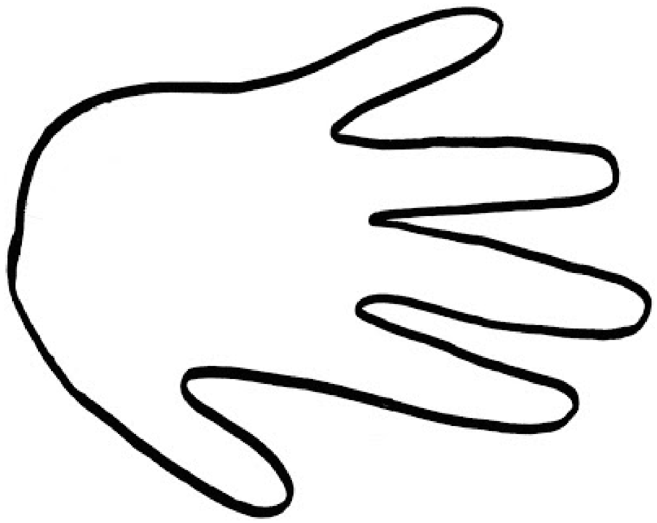
Euler characteristic

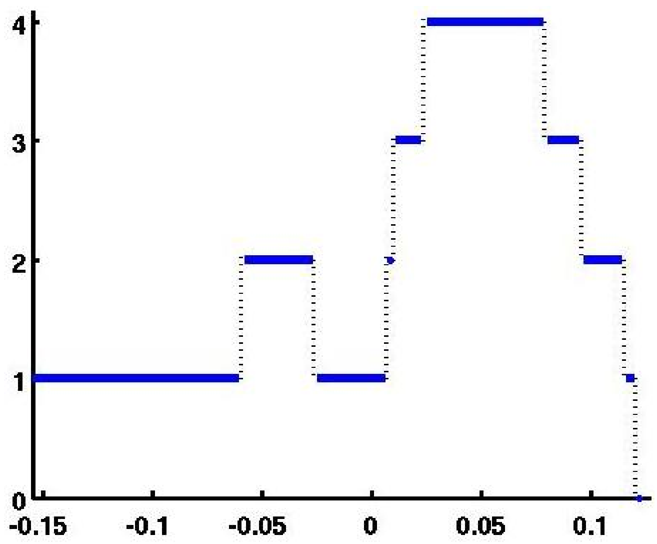
For a mesh M in 3 dimensions the Euler characteristic is

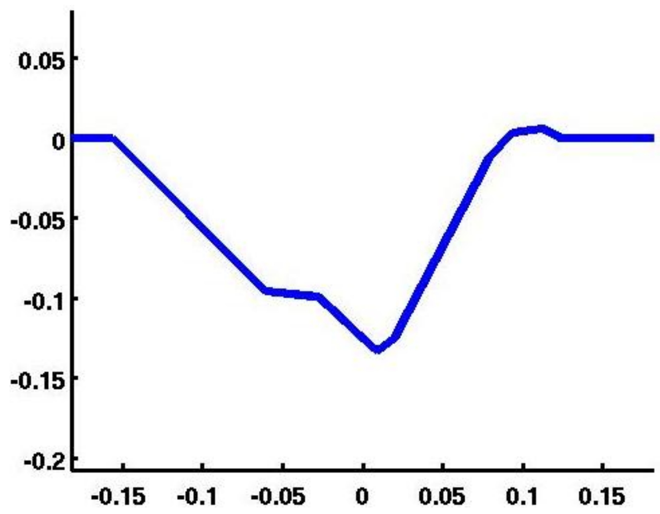
$$\chi(M) = \#\text{vertices} - \#\text{edges} + \#\text{faces}.$$



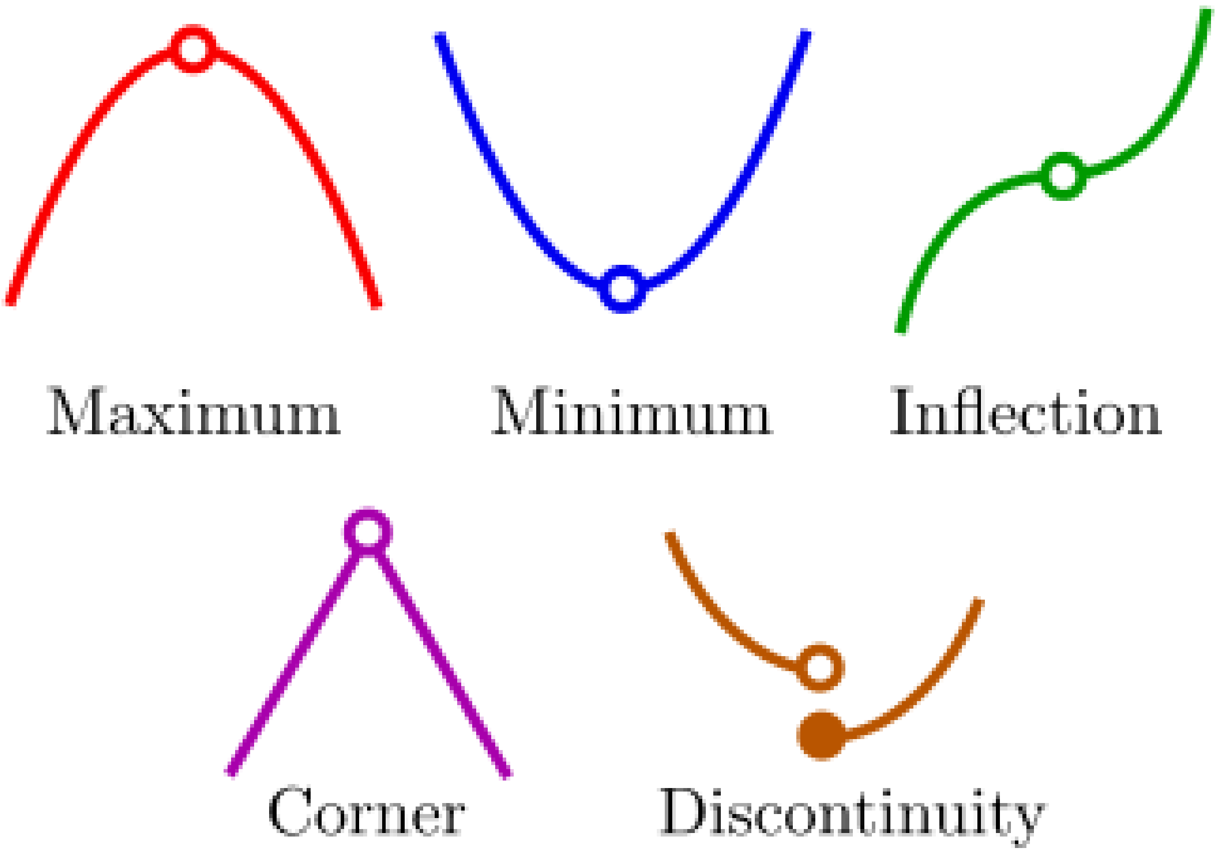
Euler characteristic curves







Critical points



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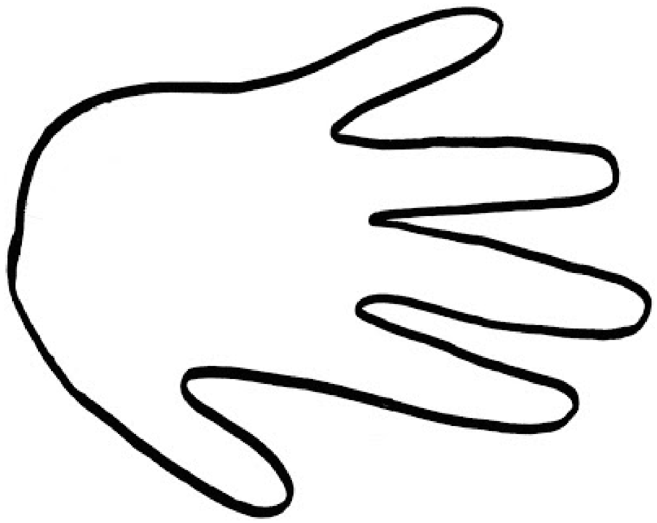
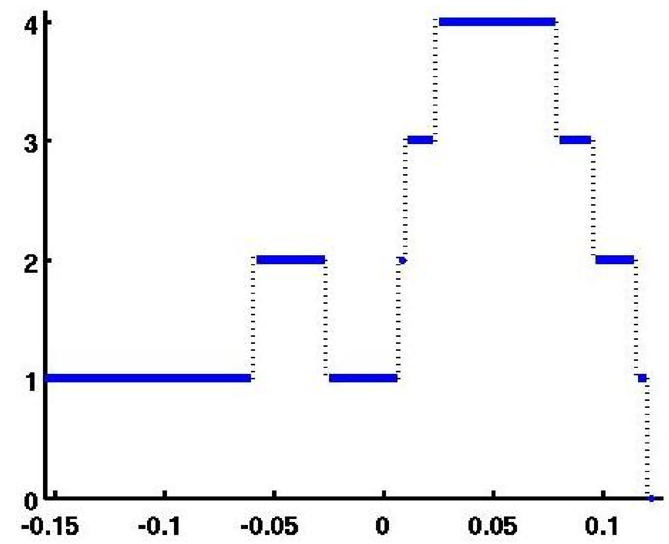
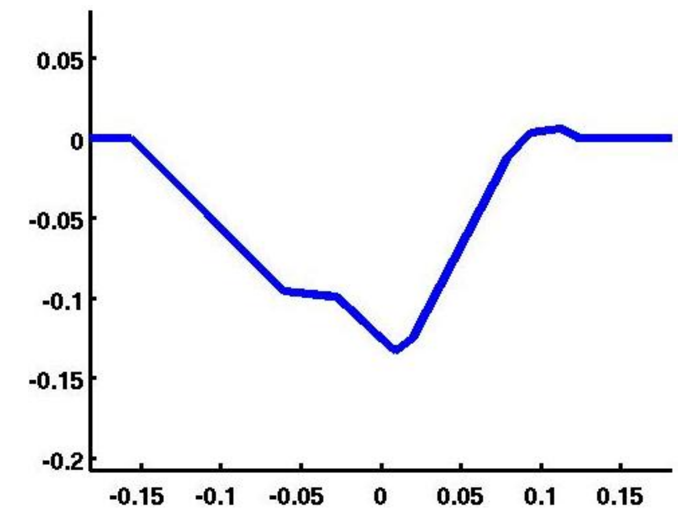
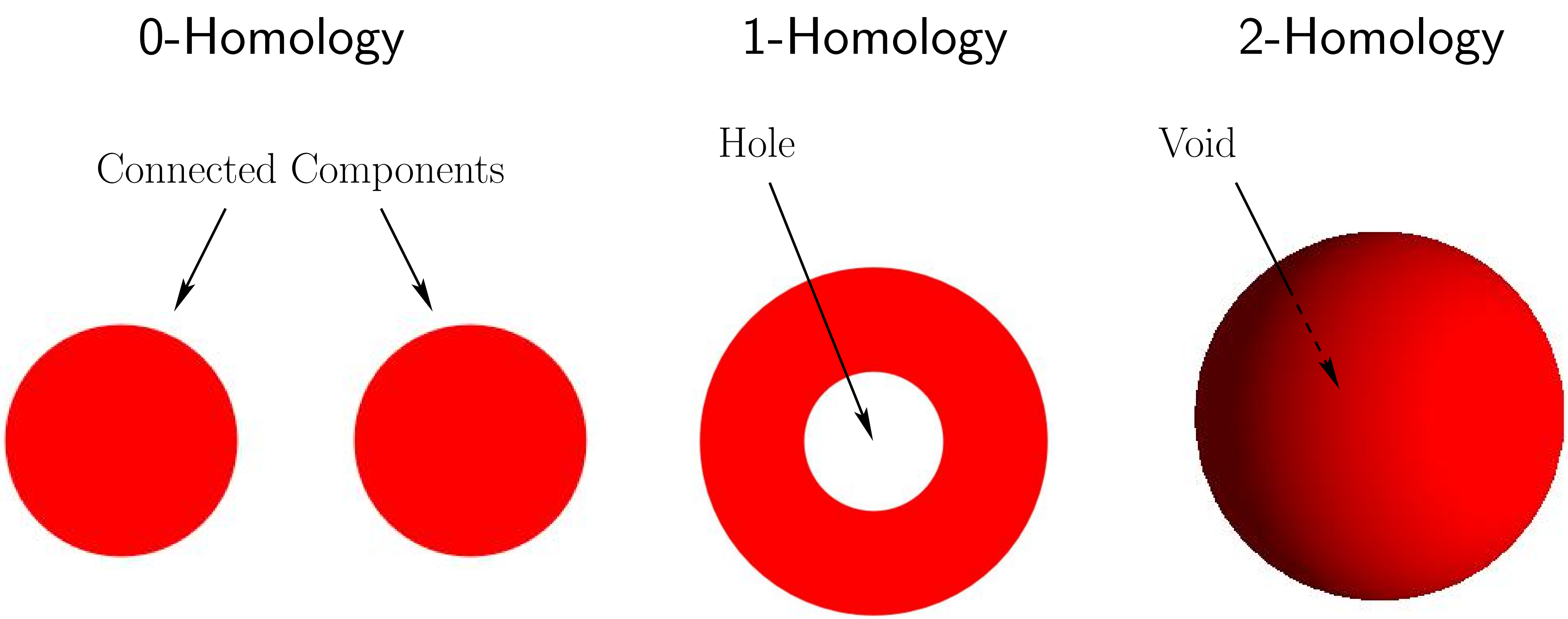






Betti numbers



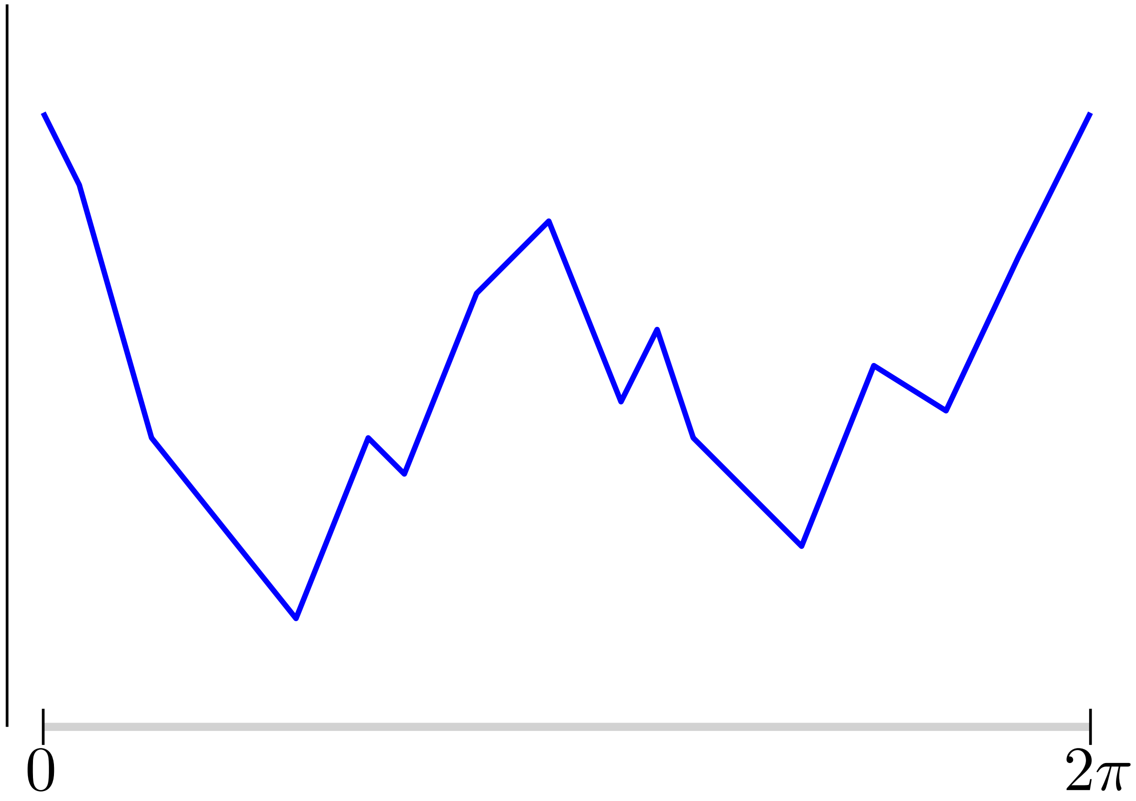
$\beta_0 = 2,\ \beta_1 = 0,\ \beta_2 = 0$

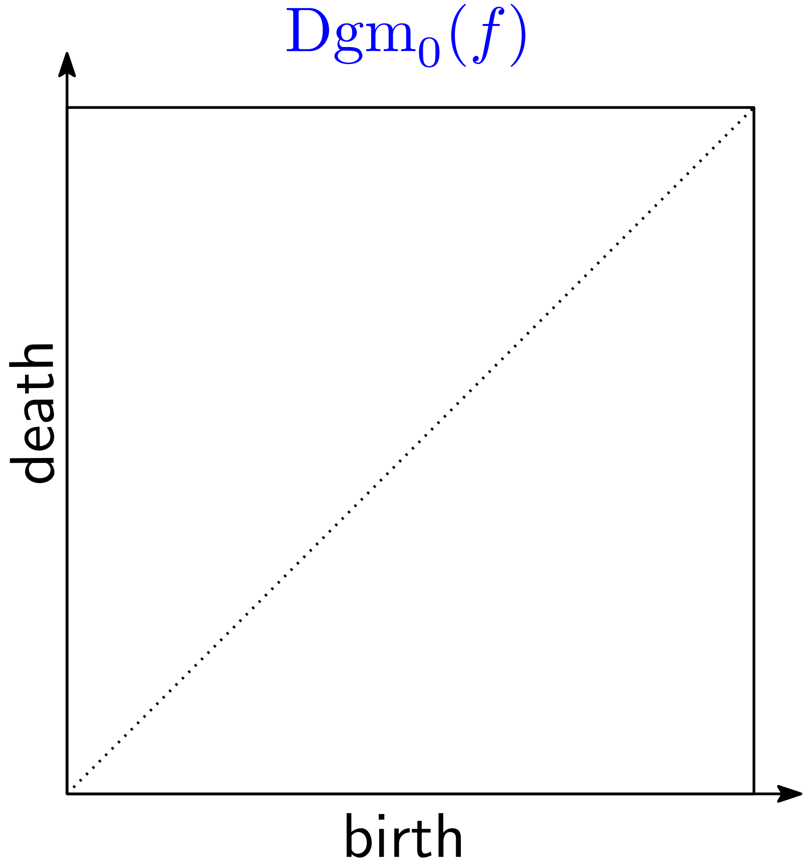
$\beta_0 = 1,\ \beta_1 = 1,\ \beta_2 = 0$

$\beta_0 = 1,\ \beta_1 = 0,\ \beta_2 = 1$

Persistent homology: Morse theory

Evolution of homology as birth-death pair.





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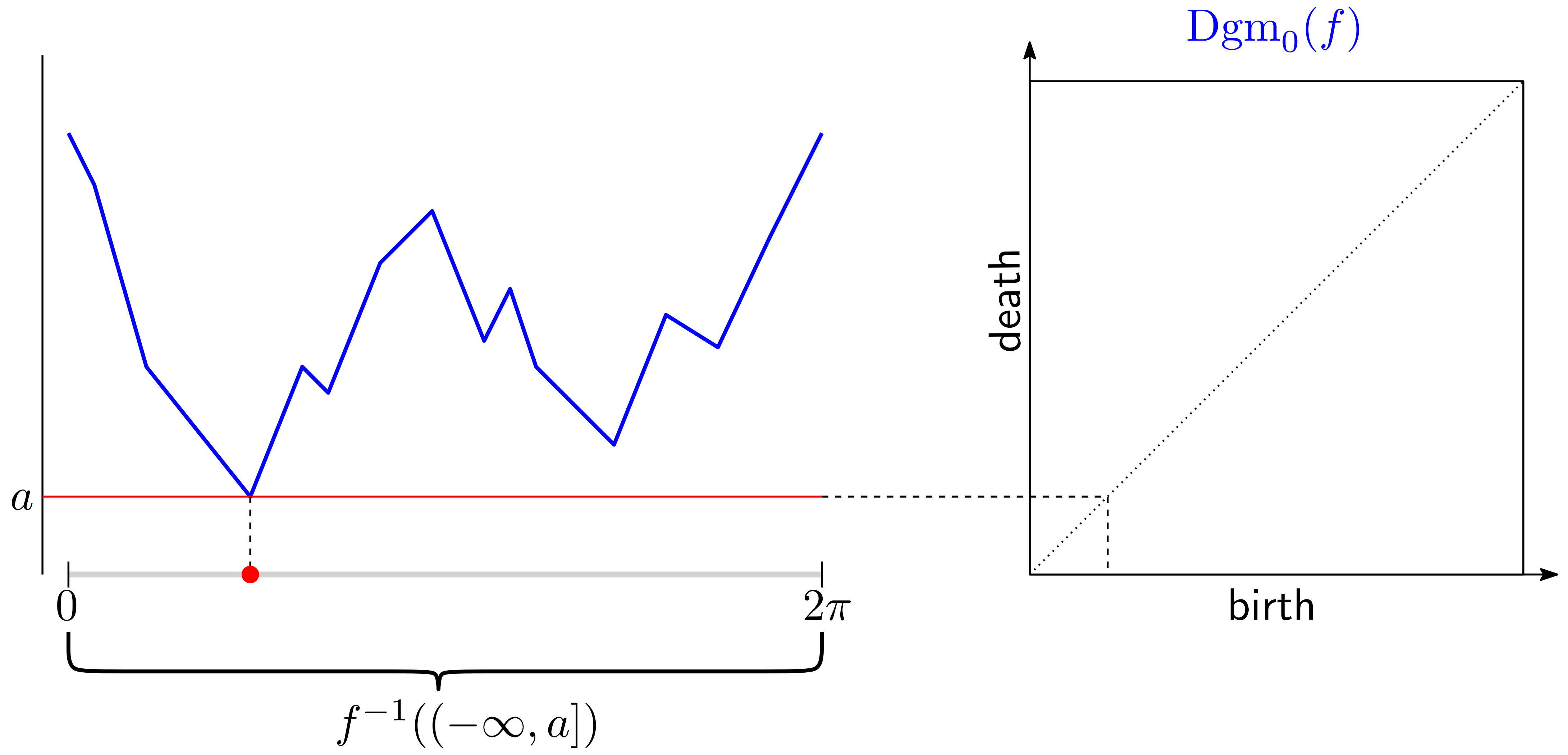

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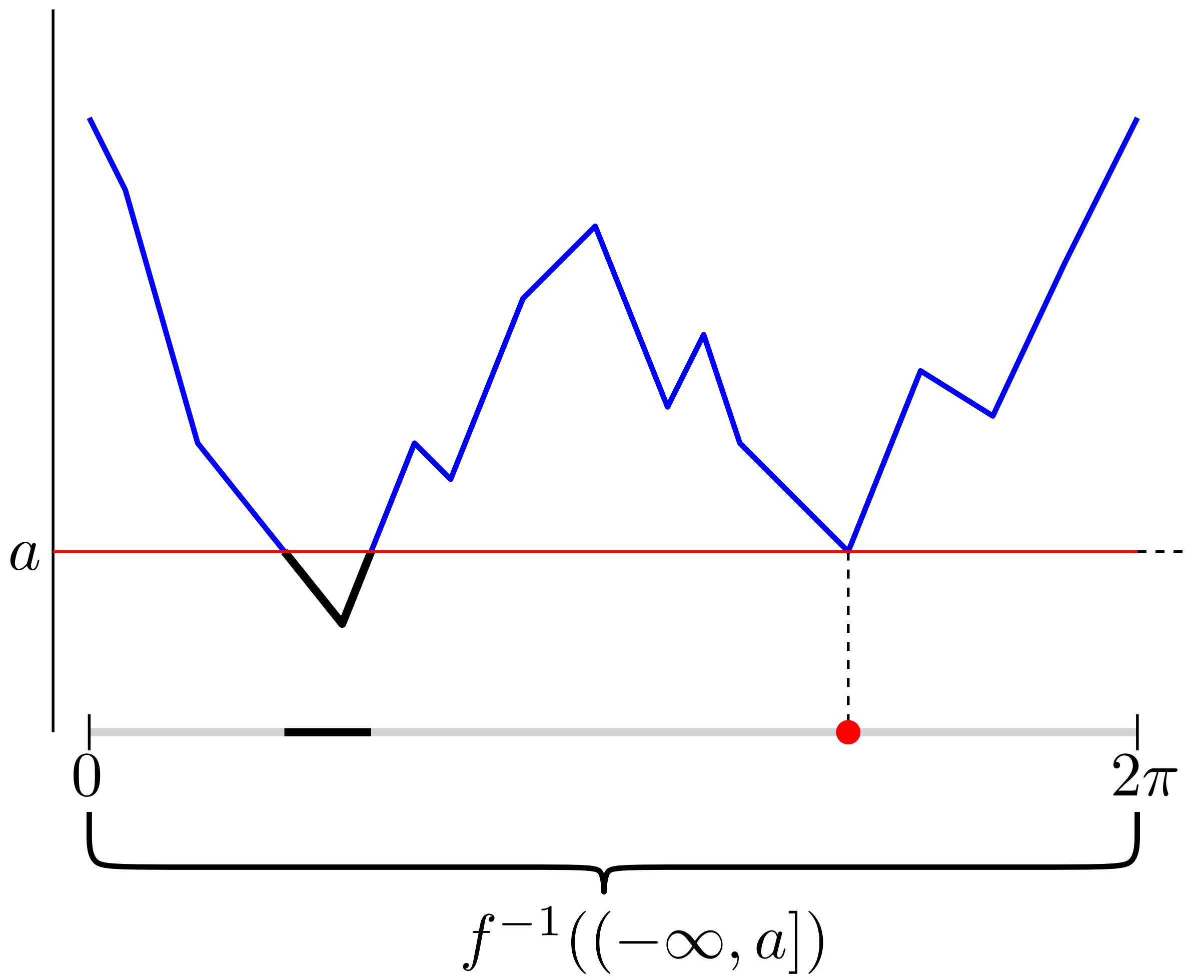

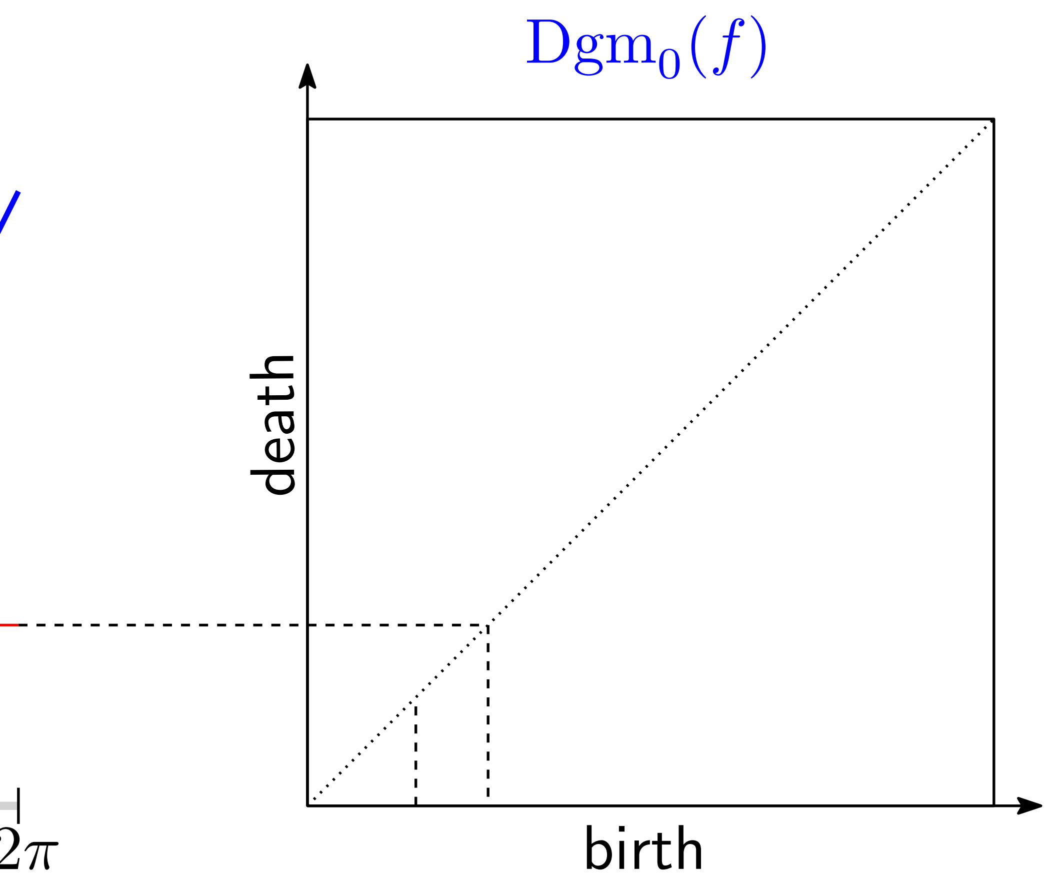

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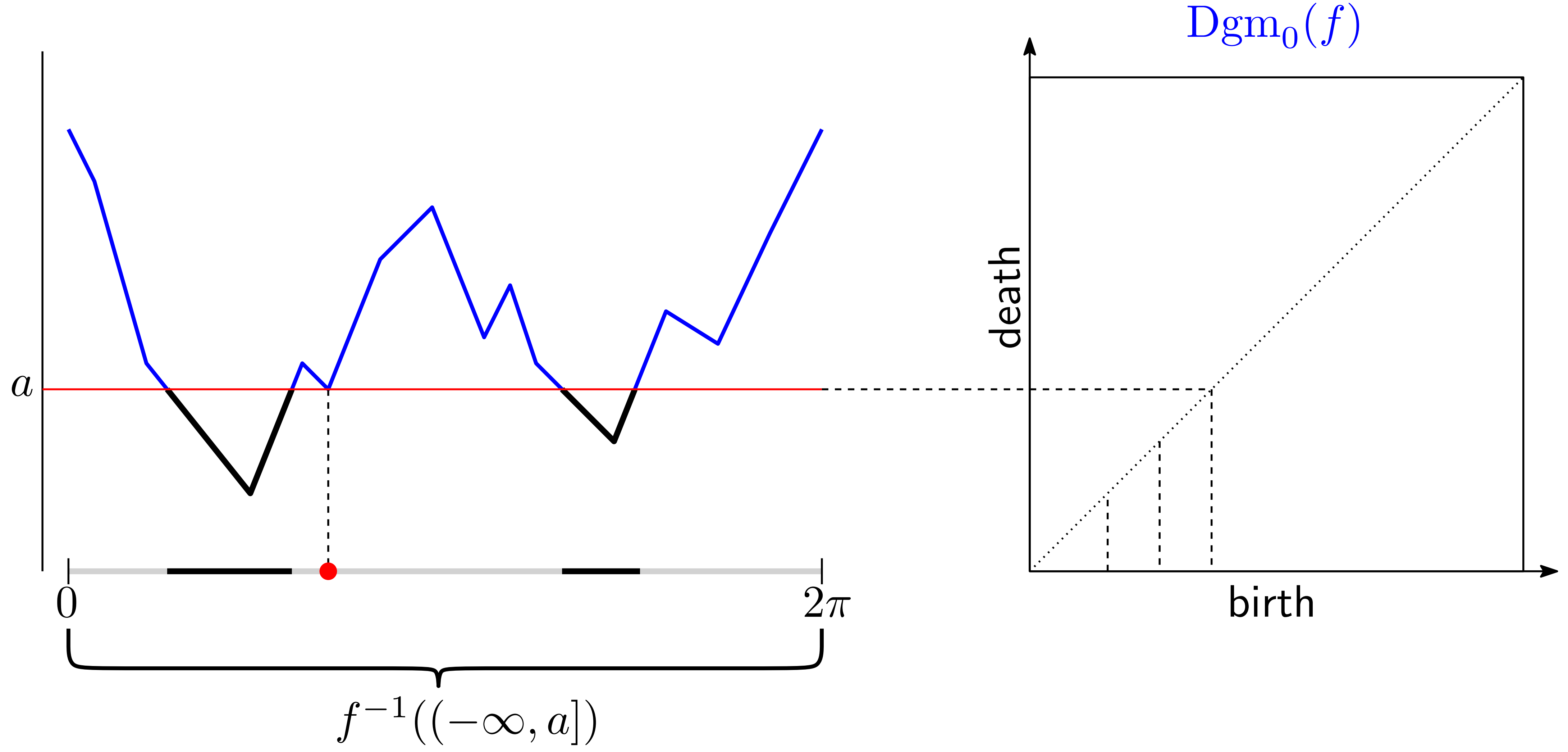

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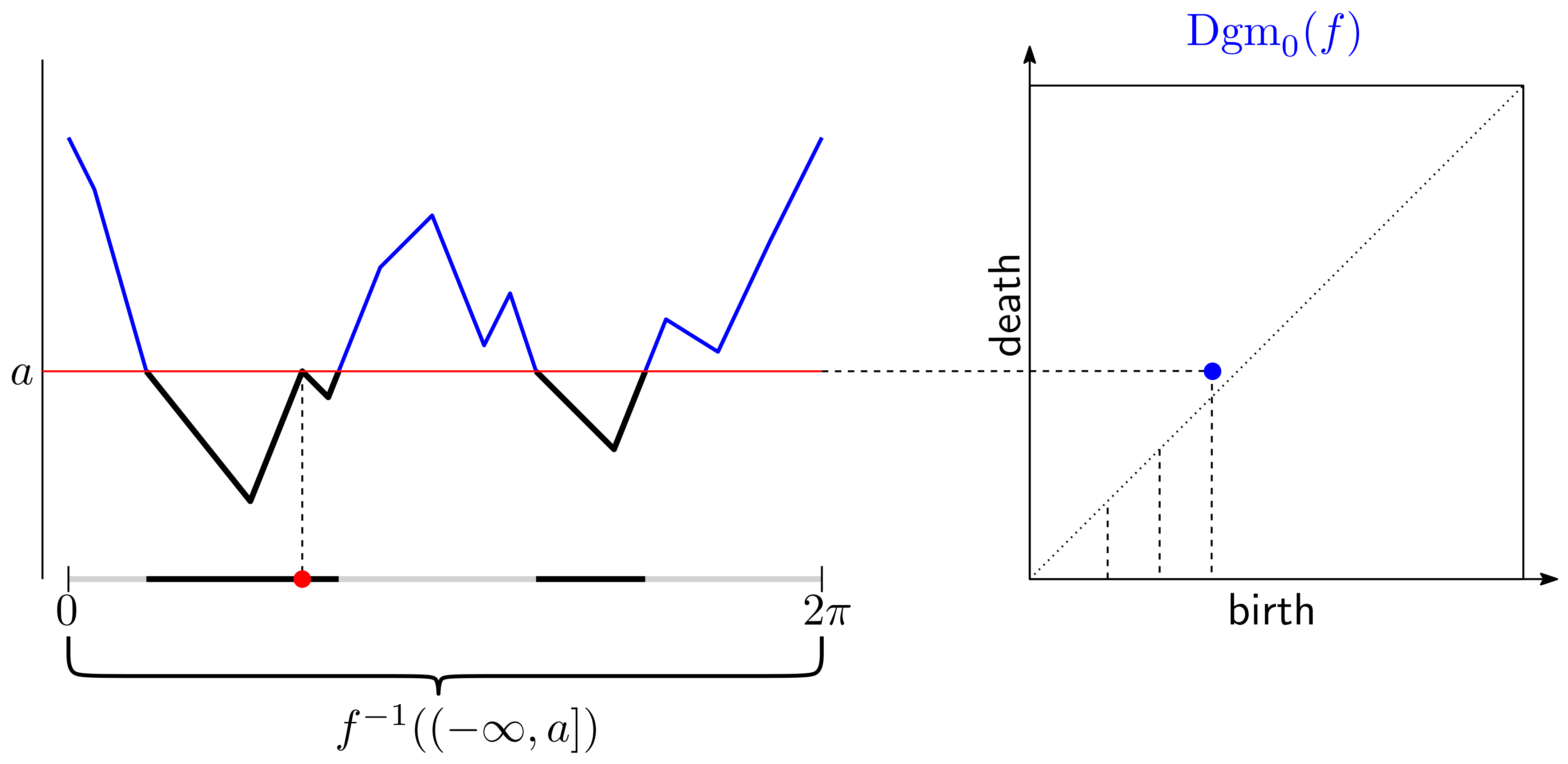

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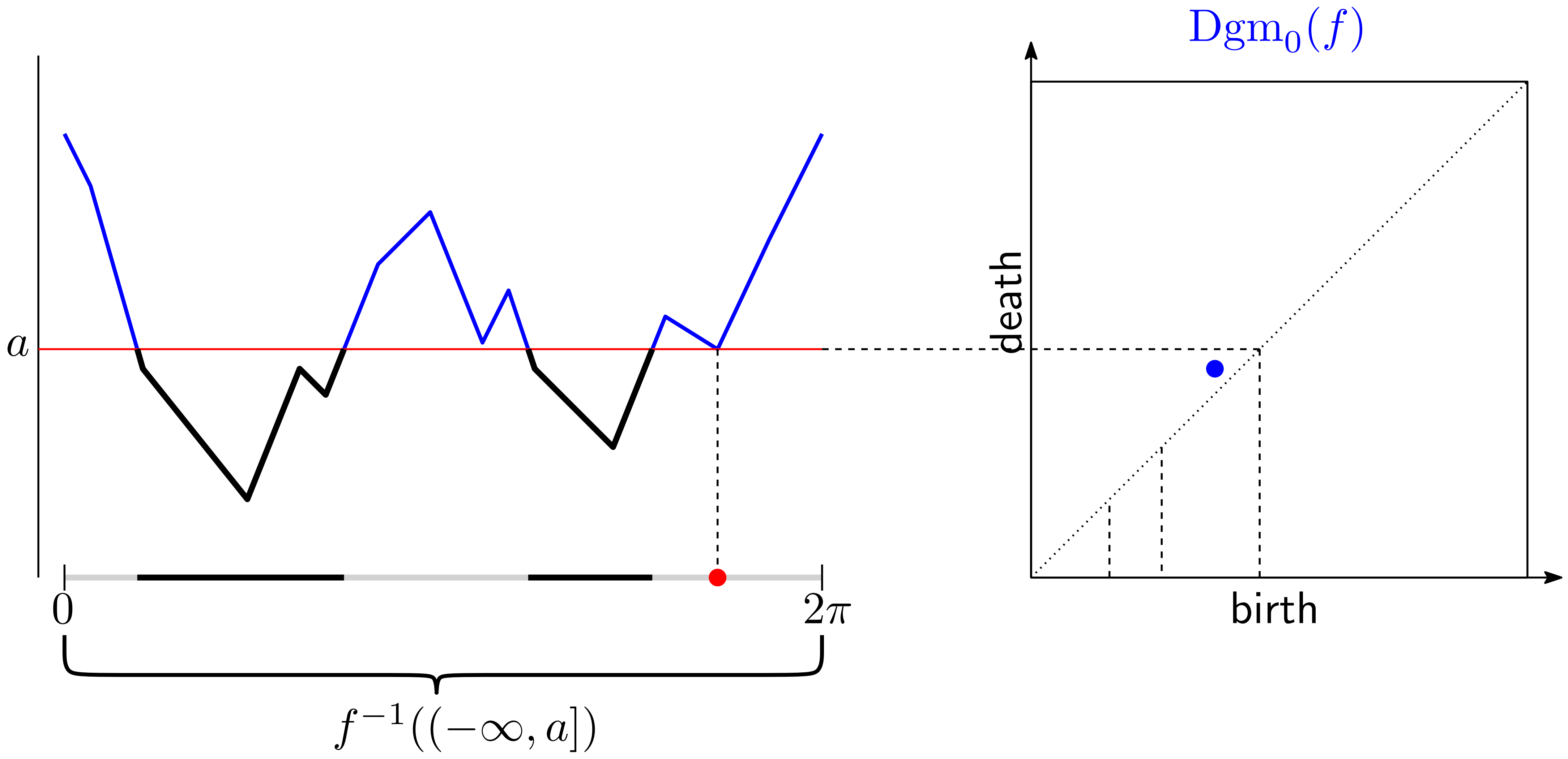

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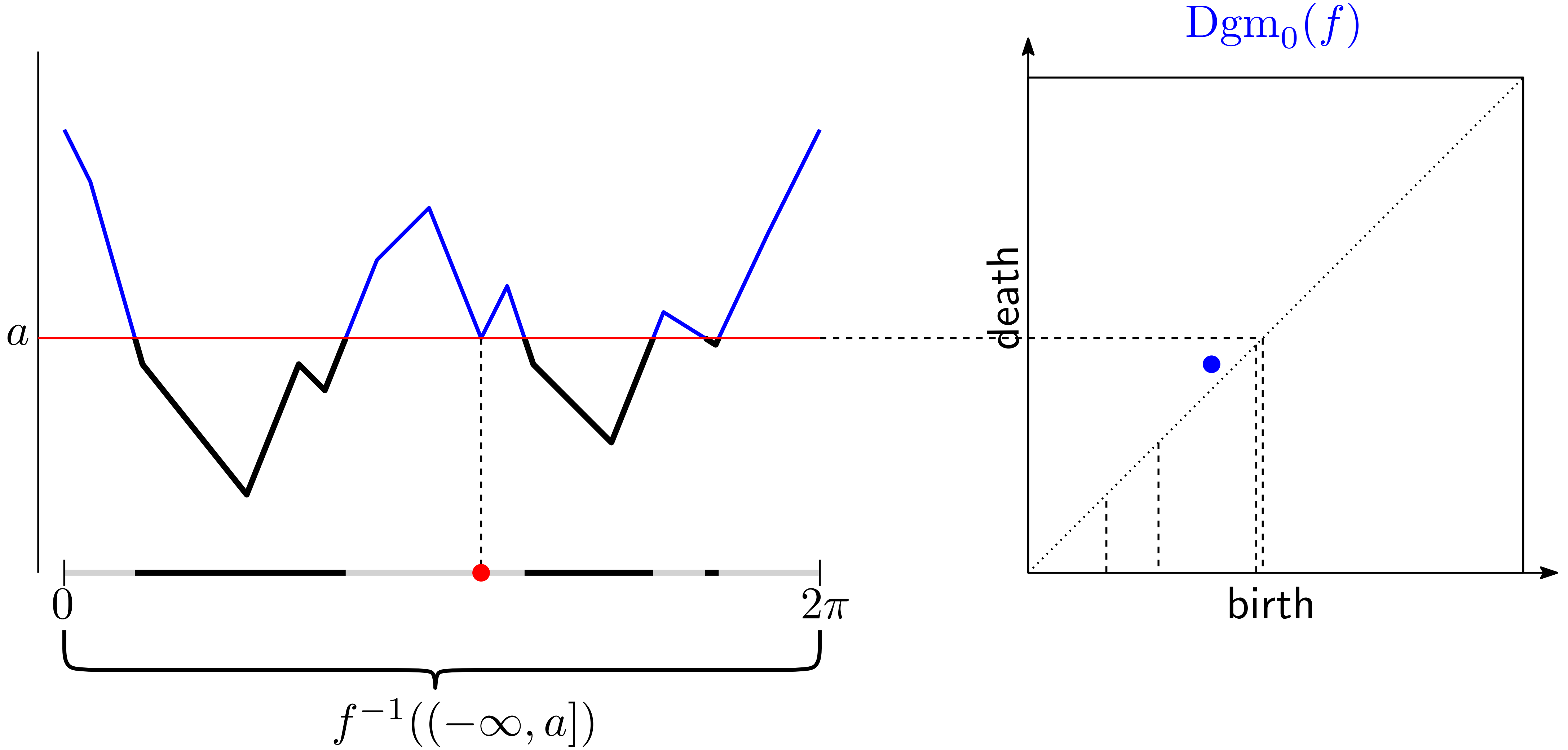

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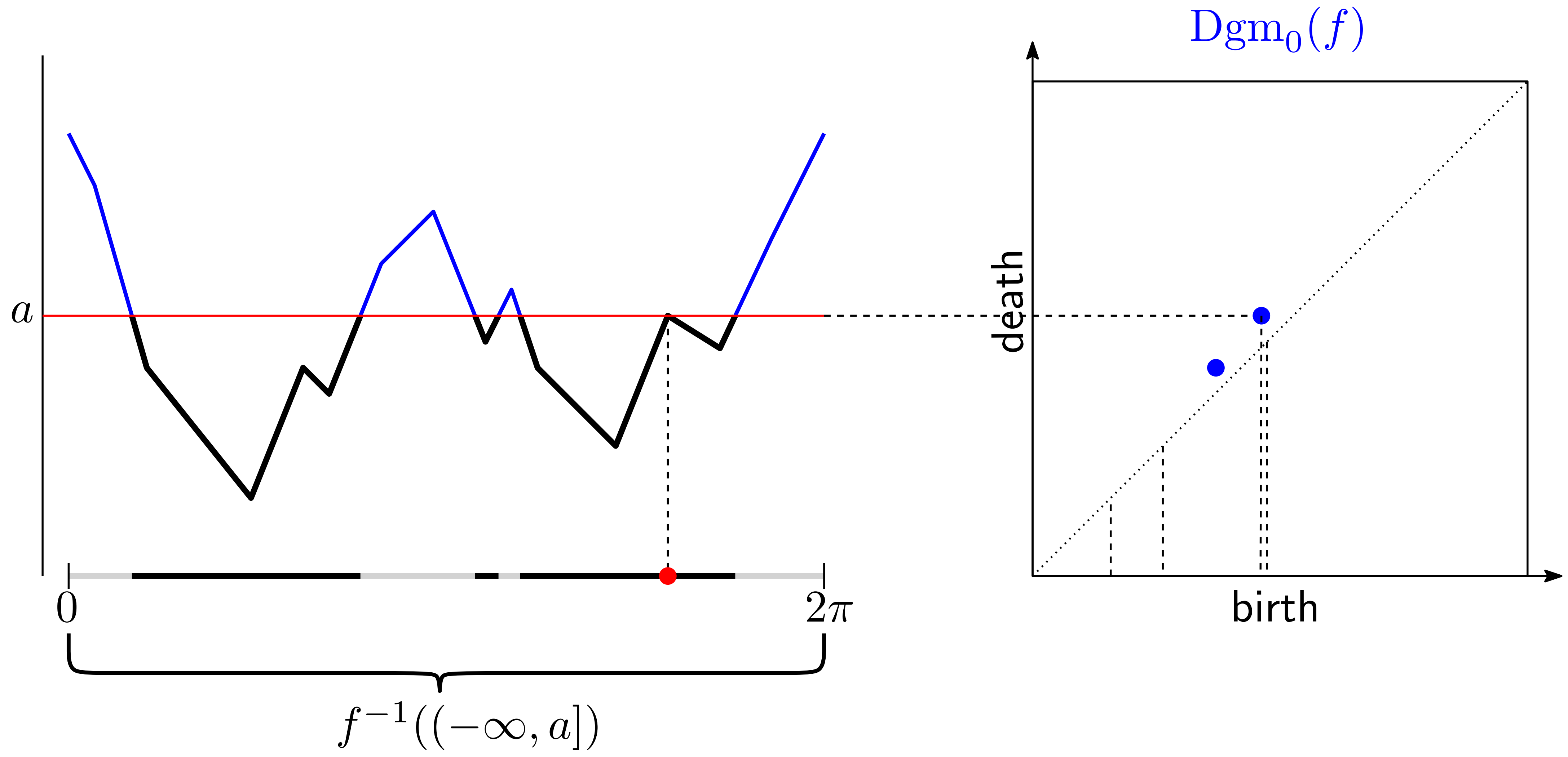

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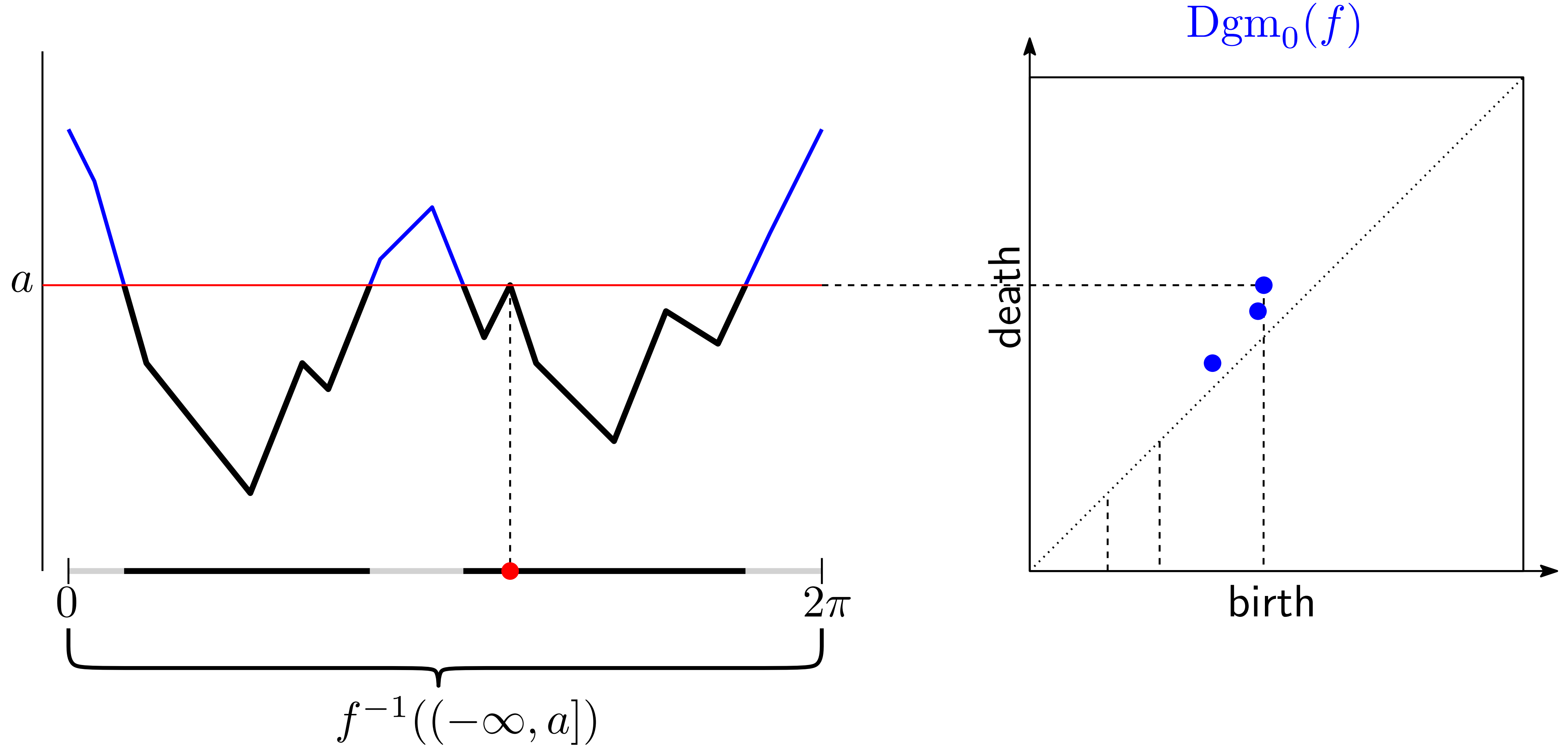

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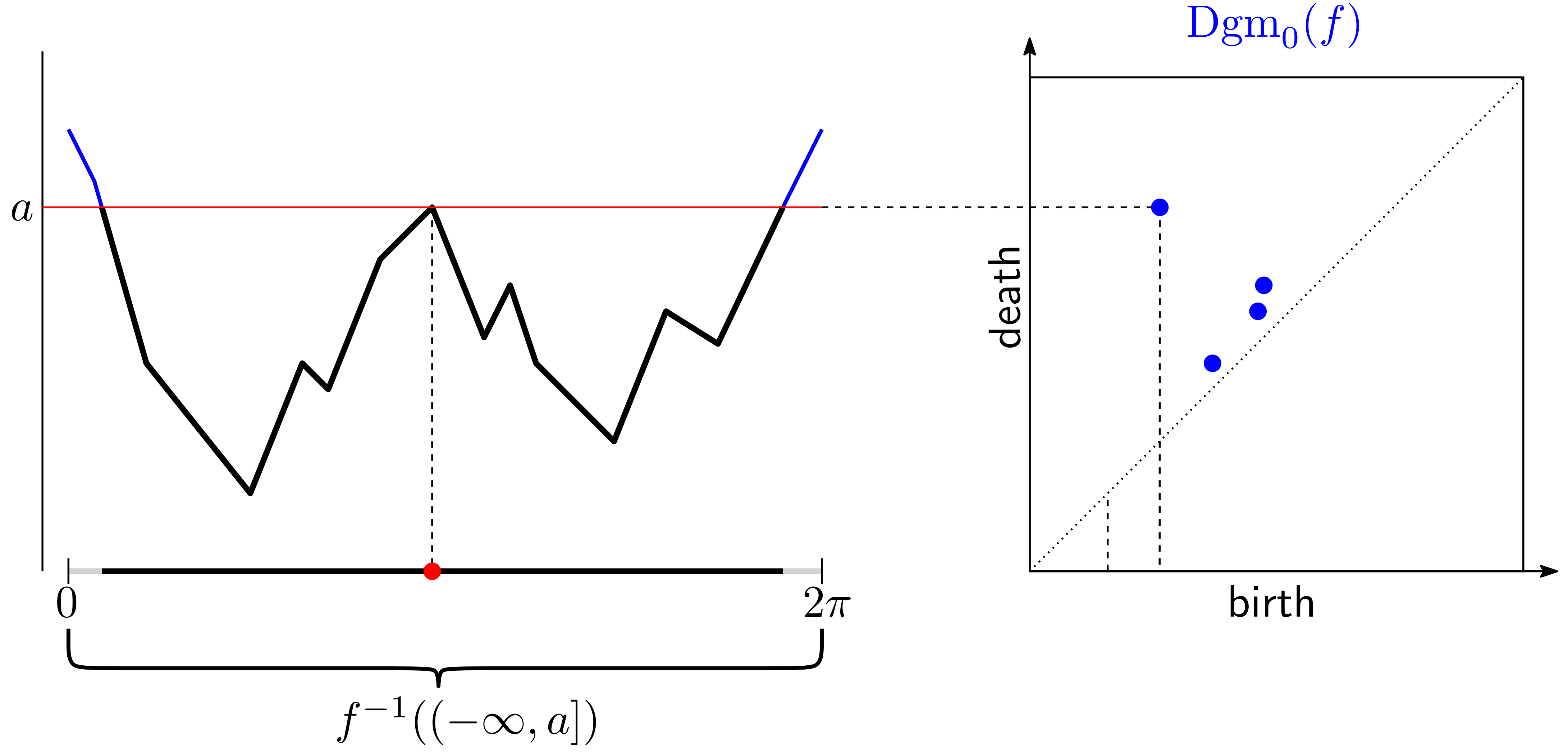

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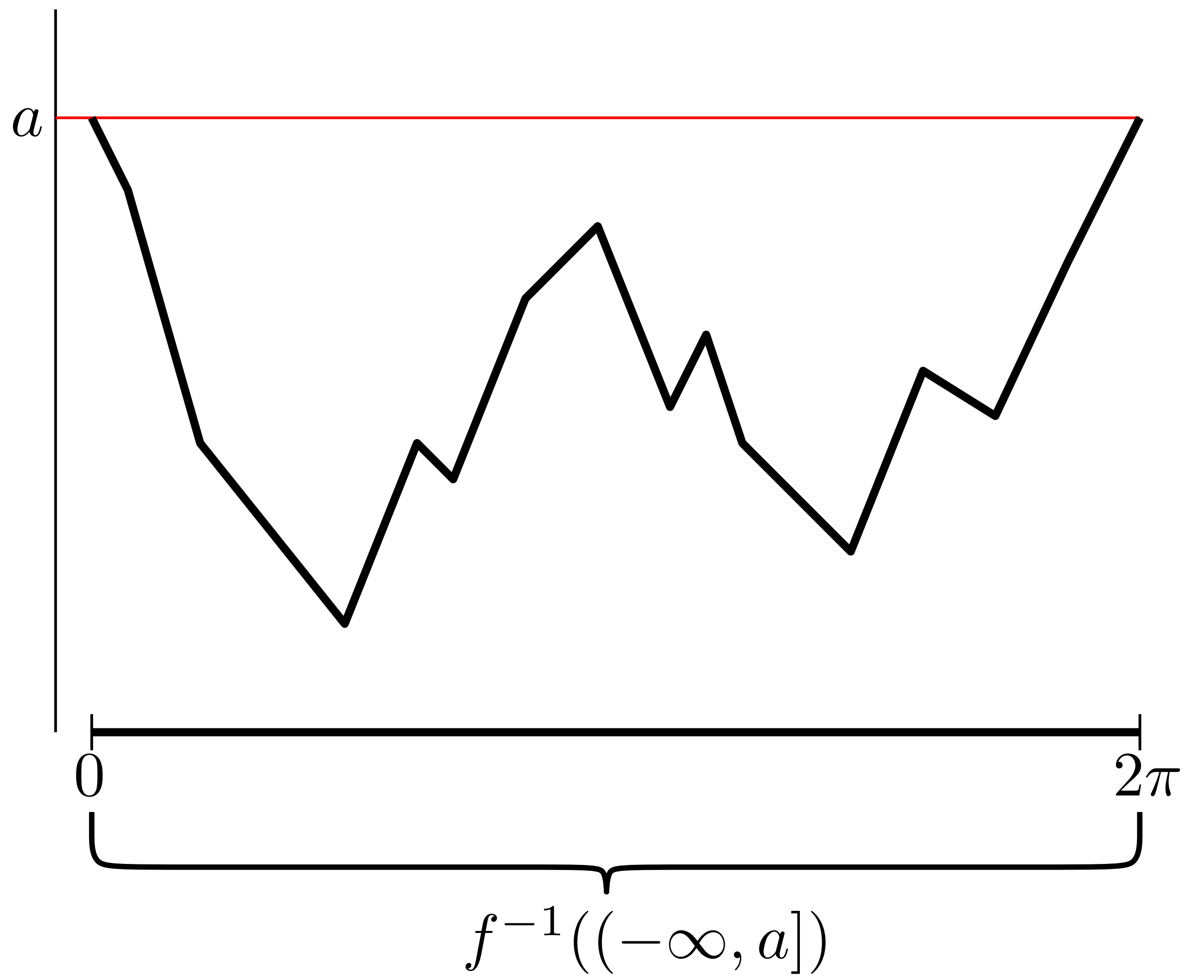

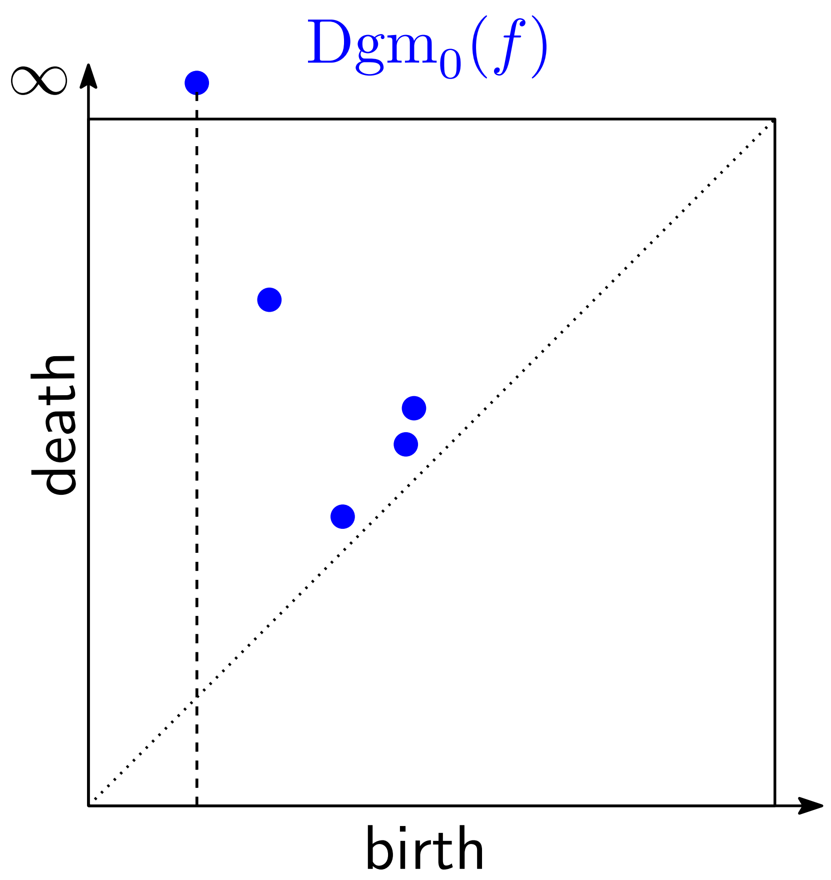

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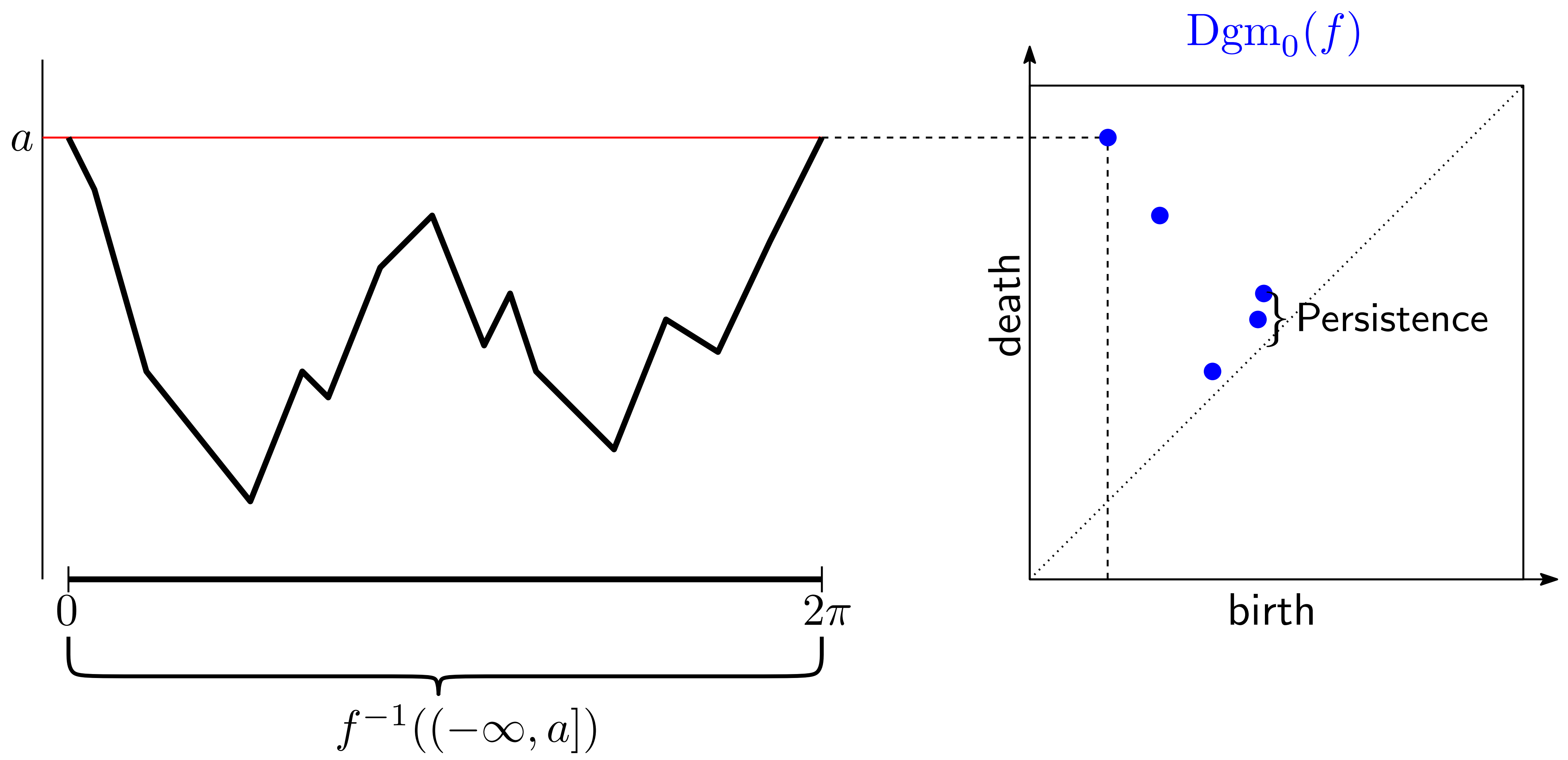
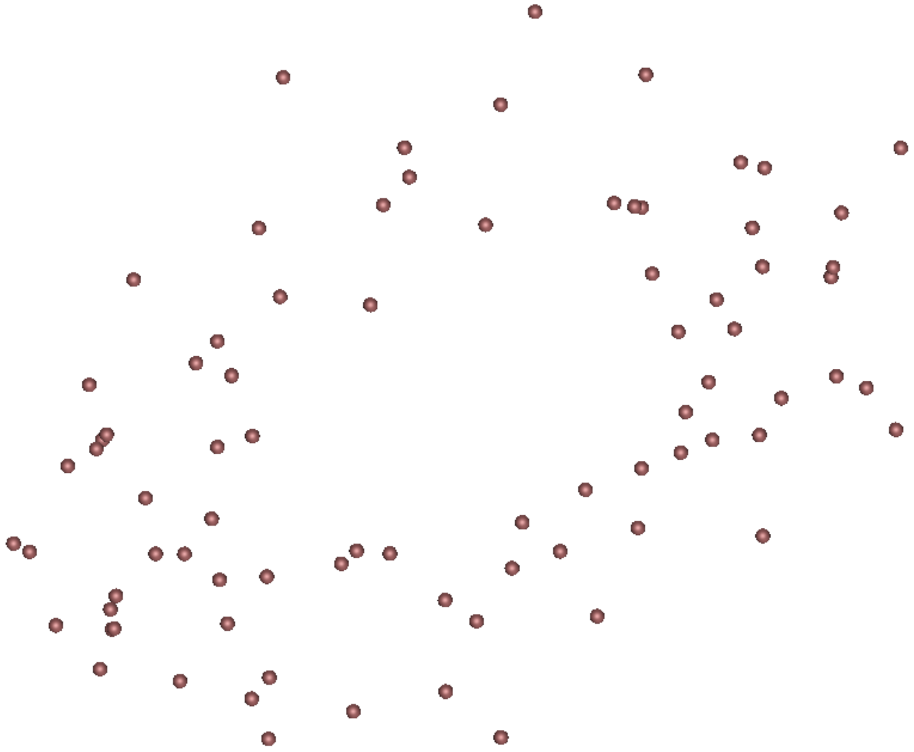
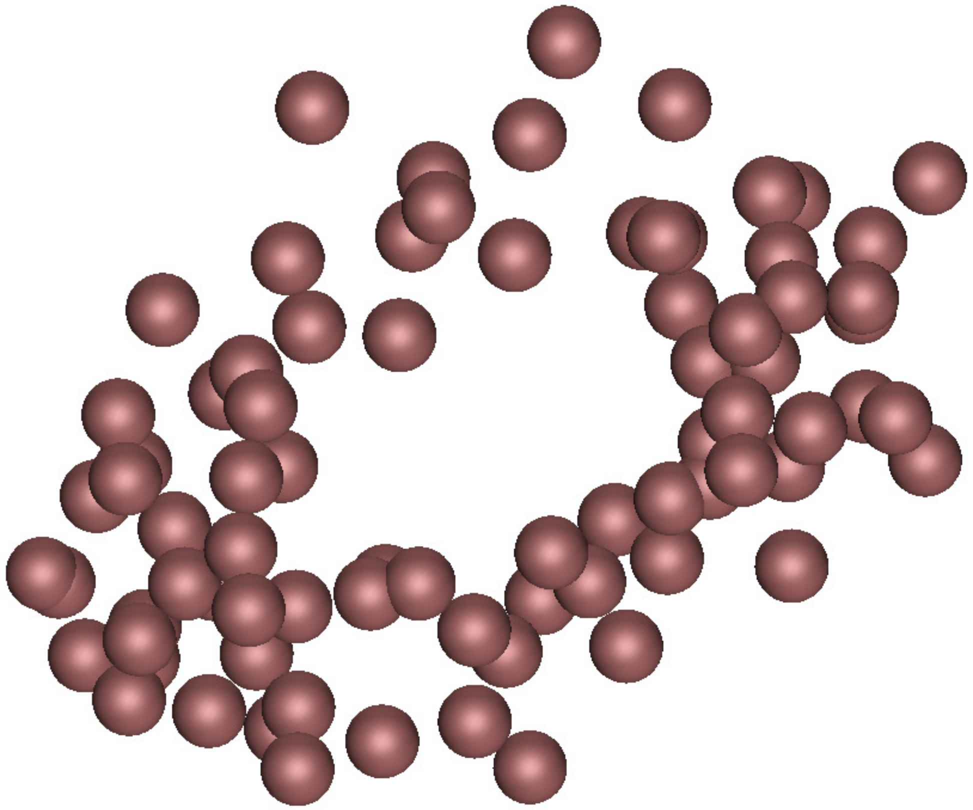


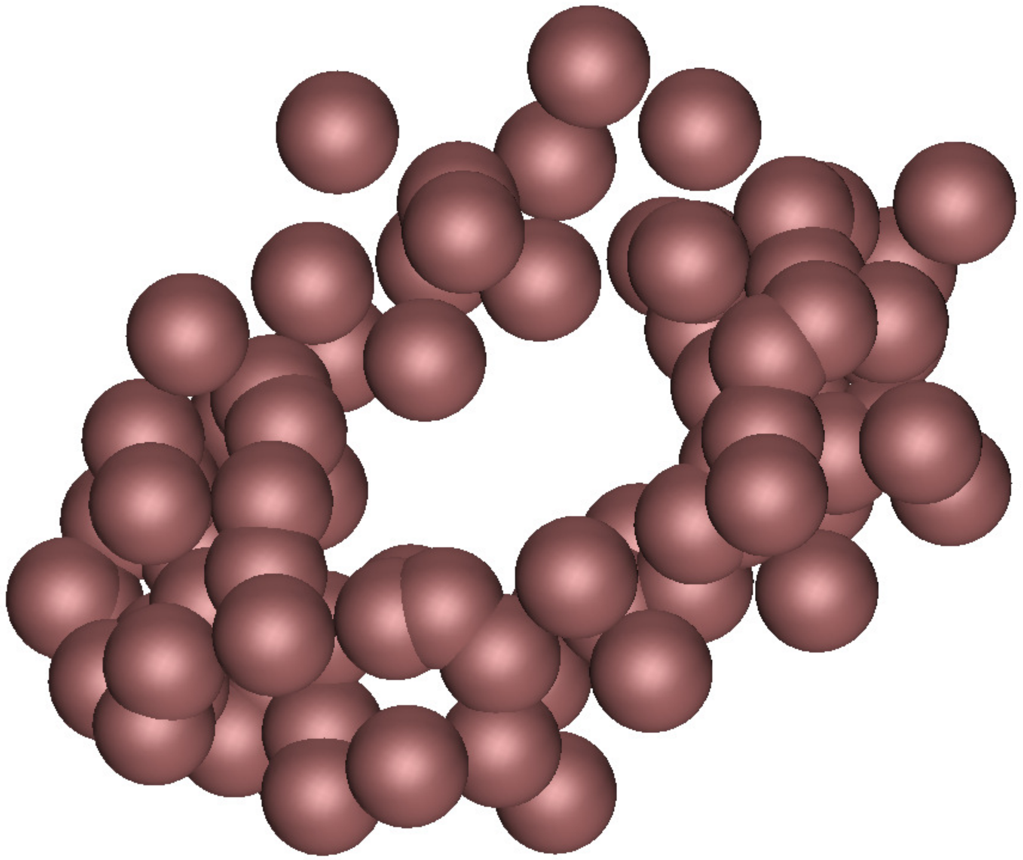
Filtration, $\mathbb{X}_0$



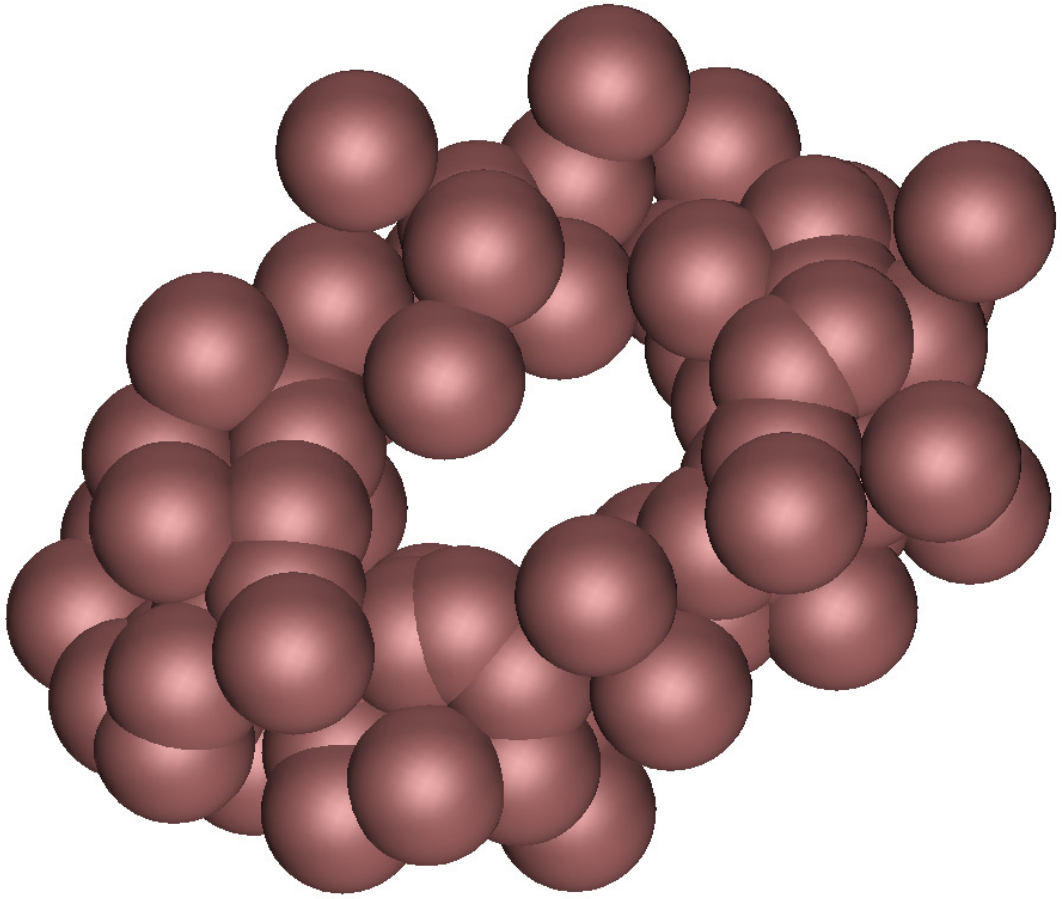
Filtration, $\mathbb{X}_1$



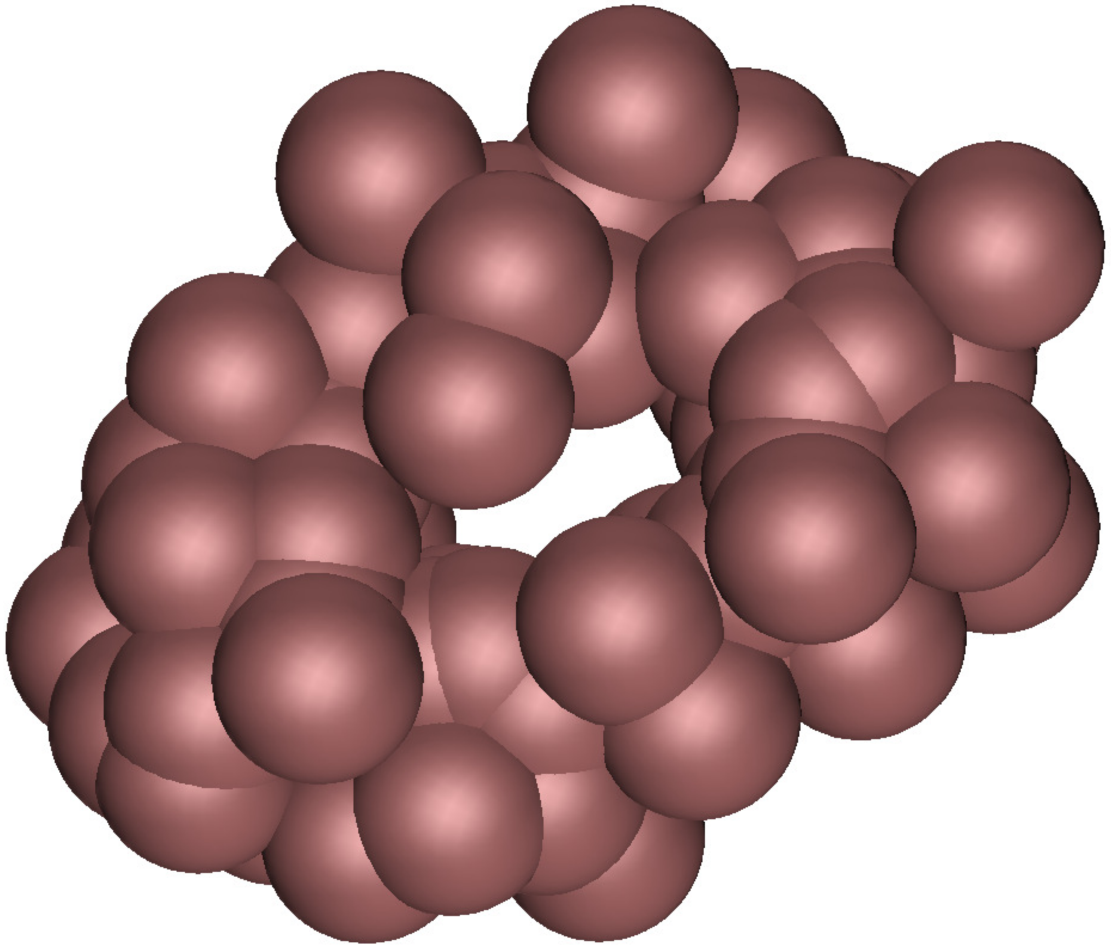
Filtration, $\mathbb{X}_2$



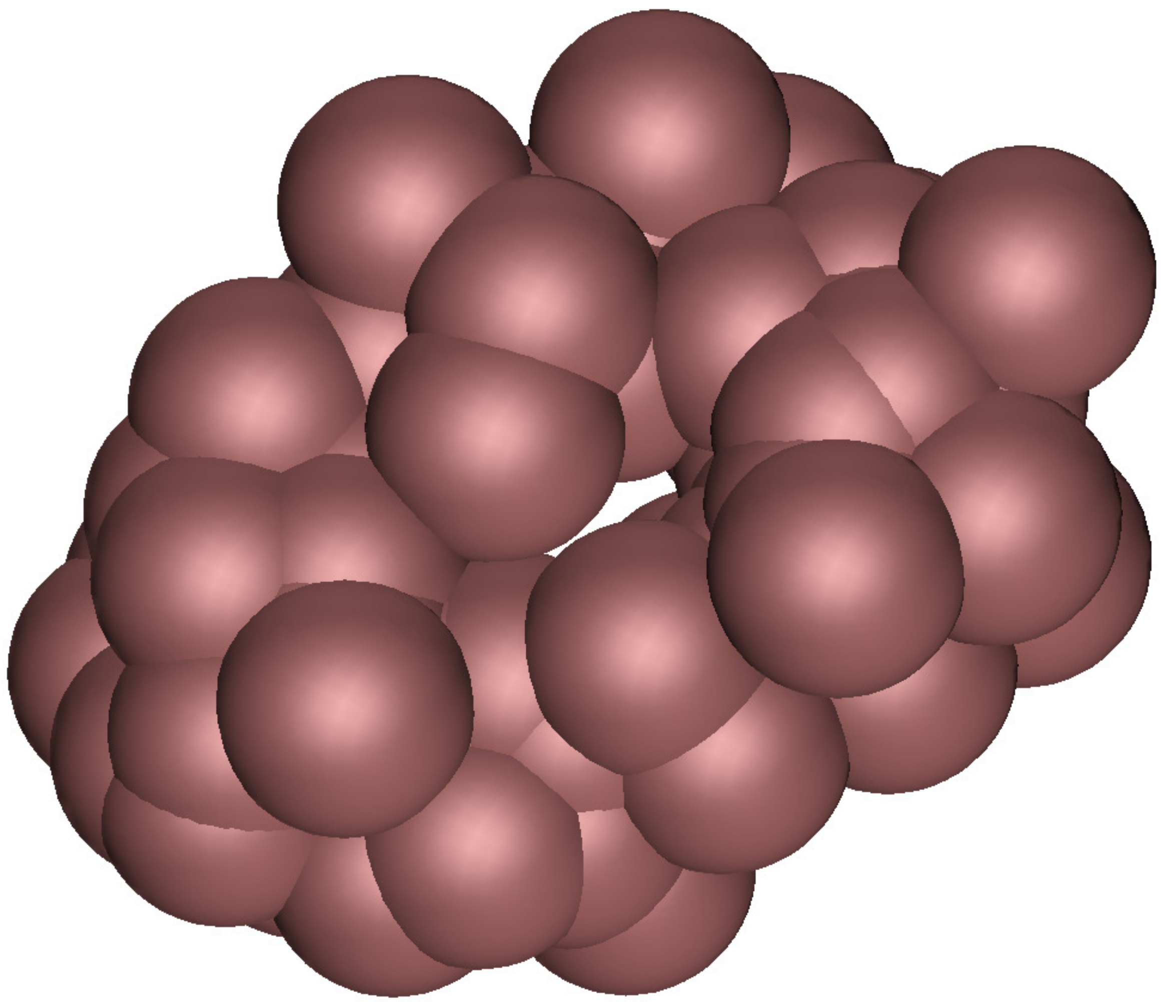
Filtration, $\mathbb{X}_3$



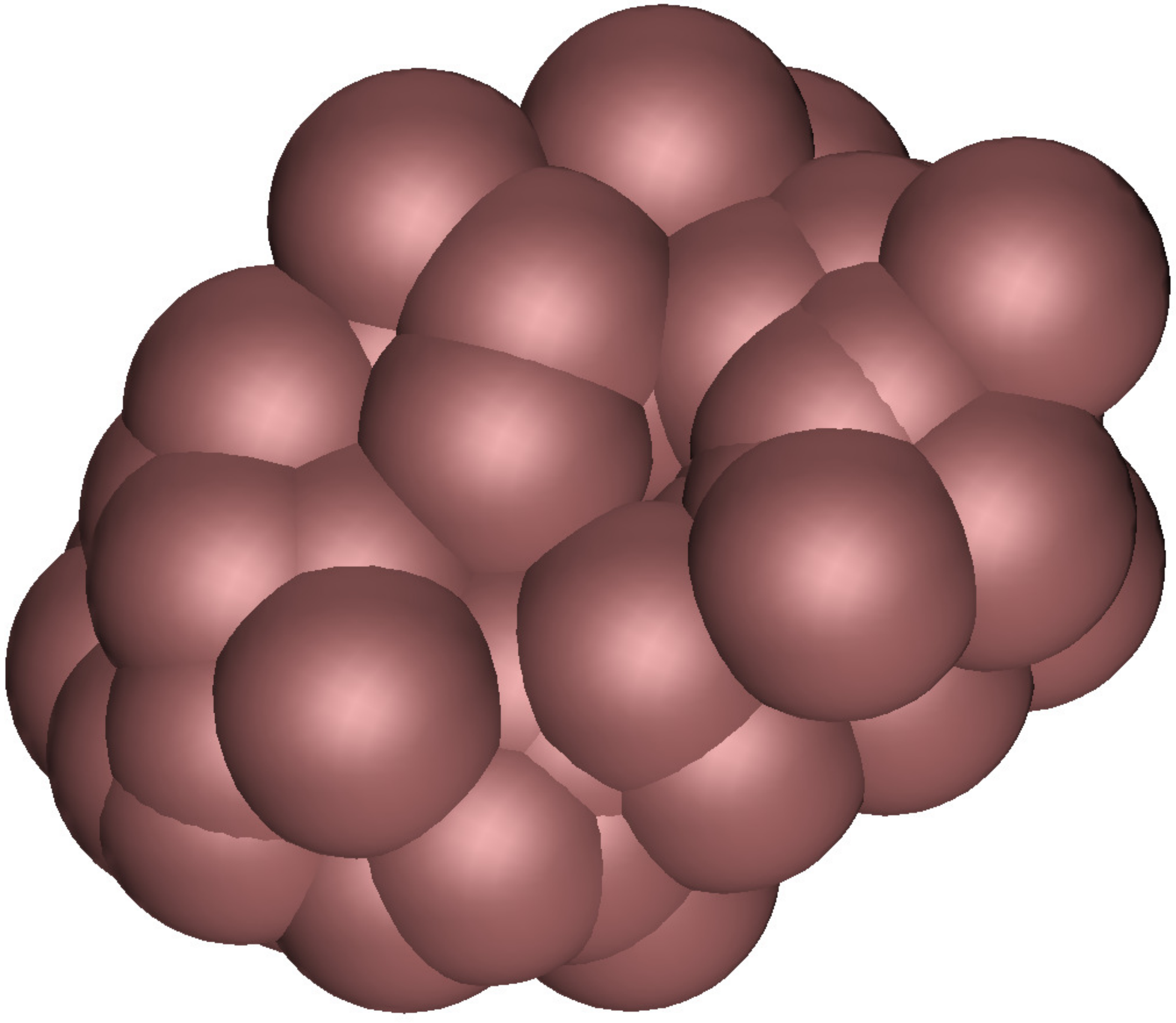
Filtration, $\mathbb{X}_4$



Filtration, $\mathbb{X}_5$

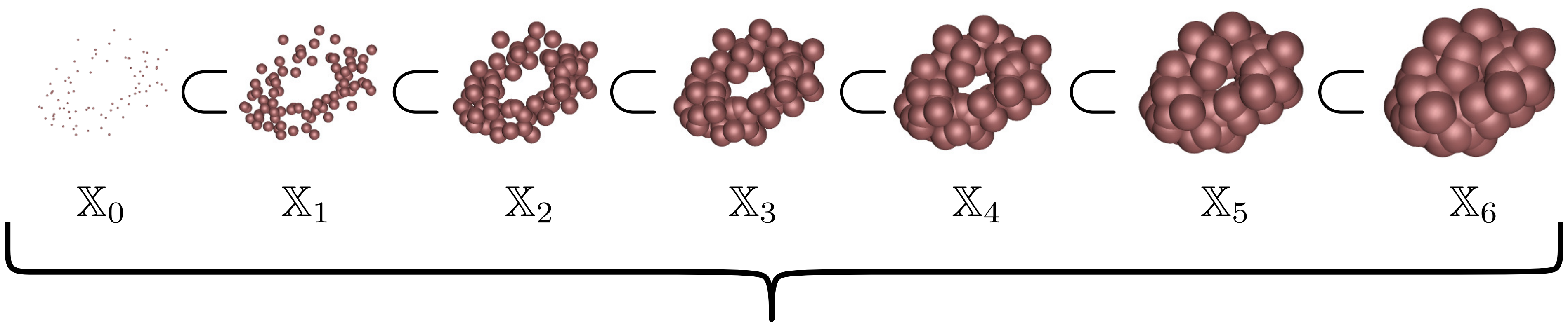


Filtration, $\mathbb{X}_6$



Persistent homology

Construct a filtration



$$H_p(\mathbb{X}_0) \to H_p(\mathbb{X}_1) \to H_p(\mathbb{X}_2) \to H_p(\mathbb{X}_3) \to H_p(\mathbb{X}_4) \to H_p(\mathbb{X}_5) \to H_p(\mathbb{X}_6)$$

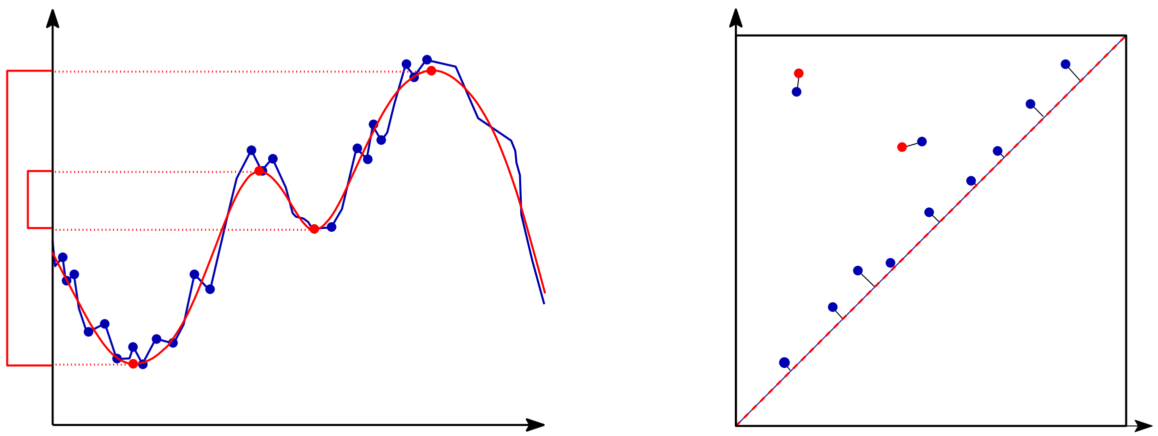
Images of linear maps $\phi_p^{i,j} : H_p(\mathbb{X}_i) \to H_p(\mathbb{X}_j)$ induced by inclusion.
Determine when a homology class is born and when it dies.

Persistence diagram

Definition

A generalized persistence diagram is a countable multiset of points in $\mathbb{R}^2$ along with the diagonal $\Delta = \{(x, y) \in \mathbb{R}^2 \mid x = y\}$, where each point on the diagonal has infinite multiplicity.

Metrics on diagrams

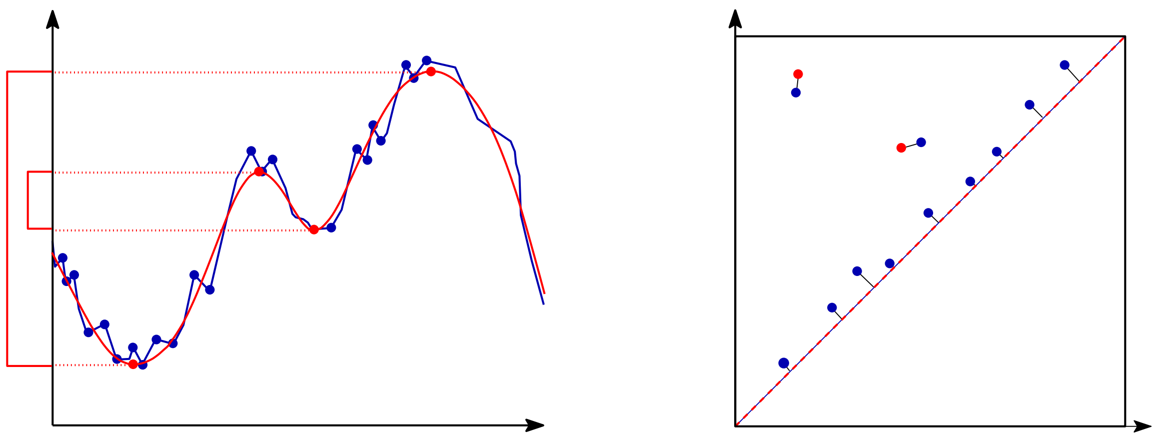


L^2-Wasserstein distance

$$d_{L^2}(X,Y)^2 = \inf_{\phi:X\to Y} \sum_{x\in X} \|x-\phi(x)\|^2,$$

ϕ is the set of bijections between the points in X plus copies of the diagonal and points in Y with copies of he diagonals.

Stability



If f, g *are tame Lipschitz functions* $f, g : \mathbb{X} \to \mathbb{R}$

$$d(Diag(f), Diag(g)) \leq 2^{\frac{k+2}{2}} \left[C \| f - g \|_\infty^{2-k} \right]^{1/2},$$

$k \in [1, 2)$.

Euler characteristic transform (ECT)

For a fixed $M \in \mathsf{CS}(\mathbb{R}^d)$ the ECT is a map from the sphere to the space of Euler curves

$$\begin{aligned} \mathsf{ECT}(M) : S^{d-1} &\to \mathsf{CF}(\mathbb{R}) \\ v &\mapsto \chi(M, v). \end{aligned}$$

where

$$\mathsf{ECT}(M)(v)(t) := \chi(M \cap \{x \mid x \cdot v \leq t\}).$$

Smooth Euler characteristic transform (SECT)

The smooth Euler curve for each direction is

$$f(y) = \chi(M, v), \quad F(x) = \int_0^x (f(y) - \overline{\chi(M, v)}) dy.$$

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Definition

The Euler characteristic transform of $M \in \mathbb{R}^d$ is the function

$$\begin{aligned} \mathrm{SECT}(M) : S^{d-1} &\to L_2(\mathbb{R}) \\ v &\mapsto F(M, v). \end{aligned}$$

Persistence homology transform (PHT)

For a fixed $M \in \mathsf{CS}(\mathbb{R}^d)$ the PHT is a map from the sphere to persistence diagrams by filtering M in the direction v

$$\begin{aligned} \mathrm{PHT}(M) : S^{d-1} &\to \mathrm{Dgm}^d \\ v &\mapsto (PH_0(M, v), PH_1(M, v), \dots, PH_{d-1}(M, v)). \end{aligned}$$

Relation between PHT and ECT

Proposition

The persistent homology Transform determines the Euler characteristic transform, i.e. we have the following commutative diagram of maps.

$$
\begin{array}{ccc}
 & & C^0(S^{d-1}, Dgm^d) \\
 & \overset{\text{PHT}}{\nearrow} & \Big\downarrow \chi \\
CS(\mathbb{R}^d) & \xrightarrow[\text{ECT}]{} & CF(S^{d-1} \times \mathbb{R})
\end{array}
$$

Distances

The distance between two shapes $M_1, M_2 \in \mathrm{CS}(\mathbb{R}^d)$ can be

$$d(M_1, M_2) \quad := \quad \int_{S^{d-1}} \|F(M_1, v) - F(M_2, v)\|_2 \, d\nu(v).$$

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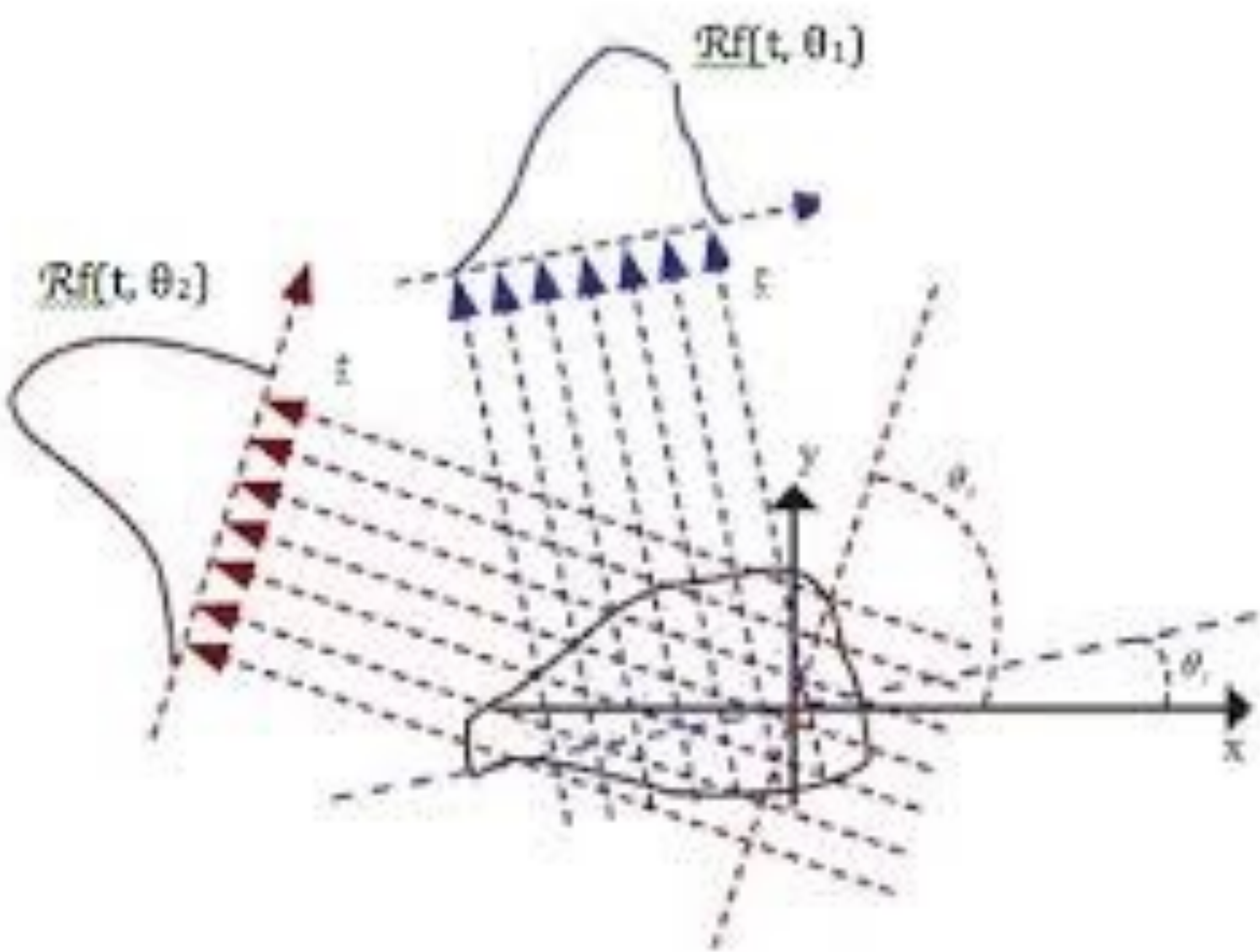
d(M_1, M_2) &:= \int_{S^{d-1}} \|F(M_1, v) - F(M_2, v)\|_2 \, d\nu(v). \\
d(M_1, M_2) &:= \sum_{k=0}^{d} \int_{S^{d-1}} d(PH_k(M_1, v), PH_k(M_1, v)) d\nu(v).
\end{aligned}
$$

Radon transform



Inversion theorem (Schapira)

Theorem (Schapira 1991)

If $S \subset X \times Y$ and $S' \subset Y \times X$ have fibers S_x and S'_x in Y satisfying

1. $\chi(S_x \cap S'_x) = \chi_1$ *for all* $x \in X$, *and*
2. $\chi(S_x \cap S'_{x'}) = \chi_2$ *for all* $x' \neq x \in X$,

then for all $\phi \in CF(X)$,

$$(\mathcal{R}_{S'} \circ \mathcal{R}_S)\phi = (\chi_1 - \chi_2)\phi + \chi_2 \left(\int_X \phi d\chi \right) 1_X .$$

Injectivity of the ECT and PHT

Theorem (Turner-M-Boyer,Curry-M-Turner, Ghrist-Levanger-Mai)

The Euler characteristic transform $CS(\mathbb{R}^d) \to CF(S^{d-1} \times \mathbb{R})$ *is injective.*

Theorem (Turner-M-Boyer,Curry-M-Turner, Ghrist-Levanger-Mai)

The persistent homology transform $CS(\mathbb{R}^d) \to C^0(S^{n-1}, Dgm^d)$ *is injective.*

A sampling theory for shapes

How many directions to sample ?

A sampling theory for shapes

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(1) For 2-D: 162 directions

(2) For 3-D: Over 700 directions.

A sampling theory for shapes

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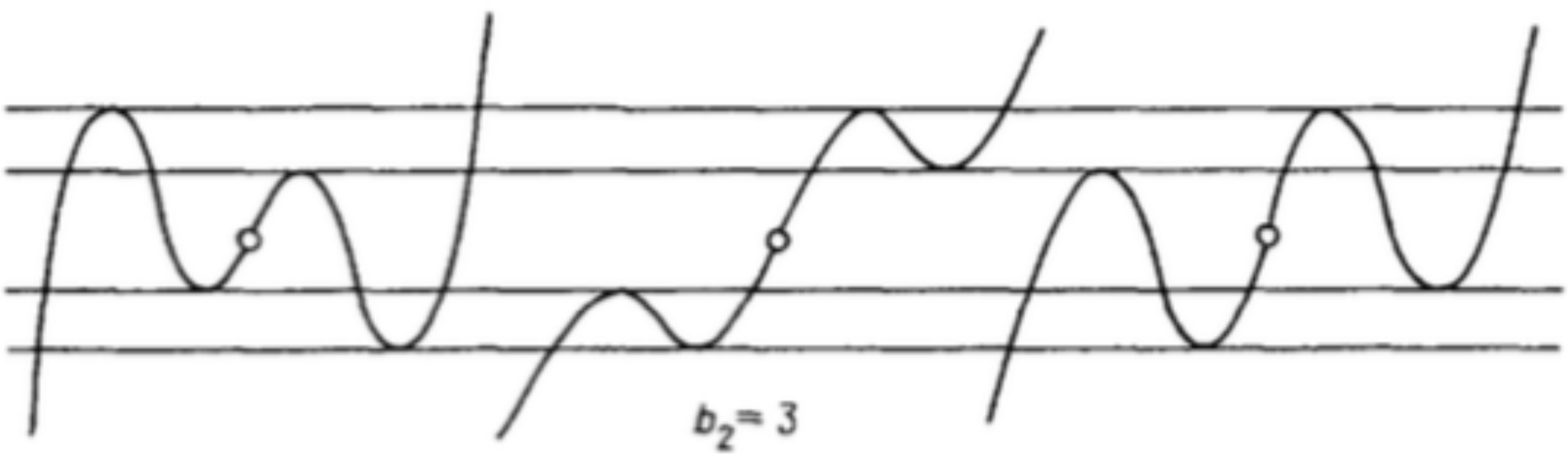
(1) For 2-D: 162 directions

(2) For 3-D: Over 700 directions.

A sampling theory for shapes — complexity metric for families shapes in terms of directions required.

Calculus of snakes

V.I. Arnol'd, The calculus of snakes and the combinatorics of Bernoulli, Euler and Springer numbers of Coxeter groups.



Moduli spaces of shapes

We now consider $\mathcal{M}(d, \delta, k)$ as the set of all embedded simplicial complexes K in $\mathbb{R}^d$ with the following two properties:

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(1) At every vertex $x \in K$ there is a lower bound on curvature δ.

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(1) At every vertex $x \in K$ there is a lower bound on curvature δ.

(2) K has at most k critical values in any direction $v \in S^{d-1}$.

Bound on the number of directions

Theorem (Curry-M-Turner)

Any shape in $\mathcal{M}(d, \delta, k)$ *can be determined using the* ECT *or the* PHT *using no more than*

$$\Delta(d, \delta, k) = \left((d-1)k \left(\frac{2\delta}{\sin(\delta)} \right)^{d-1} + 1 \right) \left(1 + \frac{2}{\delta} \right)^{d} + O\left(\frac{dk}{\delta^{d-1}} \right)^{2d}$$

directions.

Bound on the number of directions

For a resolution δ, the number of points to get a δ cover of S^{d-1} is

$$\left(1+\frac{2}{\delta}\right)^d .$$

The number of δ-covers required to determine all the vertices of K using only the Euler curves from the union of the δ-nets

$$\left((d-1)k\left(\frac{2\delta}{\sin(\delta)}\right)^{d-1}+1\right).$$

We need to bound the cardinality of $W(X)$ as the union of $\binom{|X|}{2}$ hyperplanes which is $\sum_{j=0}^{d}\binom{n(X)}{j}$.

Mixture model

In progress:

Proposition (Kirveslahti-M-Turner)

One can model shapes in $\mathcal{M}(d, \delta, k)$ based on a mixture model of Euler curves over $W(X)$.

Modeling shapes without alignment

Theorem (Curry-M-Turner)

Let K_1 and K_2 be generic geometric simplicial complexes in $\mathbb{R}^d$. Let μ be the Lebesgue measure on S^{d-1}. If

$$\mathrm{ECT}(K_1)_*(\mu) = \mathrm{ECT}(K_2)_*(\mu),$$

then there is some $\phi \in O(d)$ such that $K_2 = \phi(K_1)$.

Exponential family and SECT

Denote the Euler characteristic curve for each direction:
$f(y) = \chi(M, v)$ Define the integral of $f(y)$ as $F(x) = \int_0^x f(y)dy$.

This results in K smooth curves $\{F_1, ..., F_K\}$.

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Exponential family model

$$p_\theta(x) = a(\theta)\, h(x) \exp\left(-\sum_{k=1}^{K} \langle \theta, F_k(x) \rangle\right).$$

The matrix variate normal

Define $\mathbf{F} = [F_1 F_2 \cdots F_K]$ as a $K \times T$ matrix and

$$p(\mathbf{F} \mid \mathbf{A}, \mathbf{U}, \mathbf{V}) = \frac{\exp\left(-\frac{1}{2}\mathrm{tr}[\mathbf{V}^{-1}(\mathbf{F}-\mathbf{A})^T\mathbf{U}^{-1}(\mathbf{F}-\mathbf{A})]\right)}{(2\pi)^{KT/2}|\mathbf{V}|^{L/2}|\mathbf{U}|^{K/2}},$$

A models mean

U models covariance between curves

V models covariance between points in a curve.

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A models mean
U models covariance between curves
V models covariance between points in a curve.

The given n meshes $(M_1, \ldots, M_n)$ we can define a likelihood model

$$\mathrm{Lik}(M_1, \ldots, M_n \mid \mathbf{A}, \mathbf{U}, \mathbf{V}) = \prod_{i=1}^{n} p(\mathbf{F}(M_i) \mid \mathbf{A}, \mathbf{U}, \mathbf{V}).$$

Exponential family model for shapes

A shape is transformed into collection of the curves $\{\chi(M, v_\ell)\}_{\ell=1}^{L}$.

A natural exponential family model for the collection of these curves is a multivariate Gaussian process

$$\mathbf{X} = \begin{bmatrix} \chi(M, v_1) \\ \vdots \\ \chi(M, v_L) \end{bmatrix} \sim \mathcal{GP}_L(\mu, k).$$

Picture of heel bone

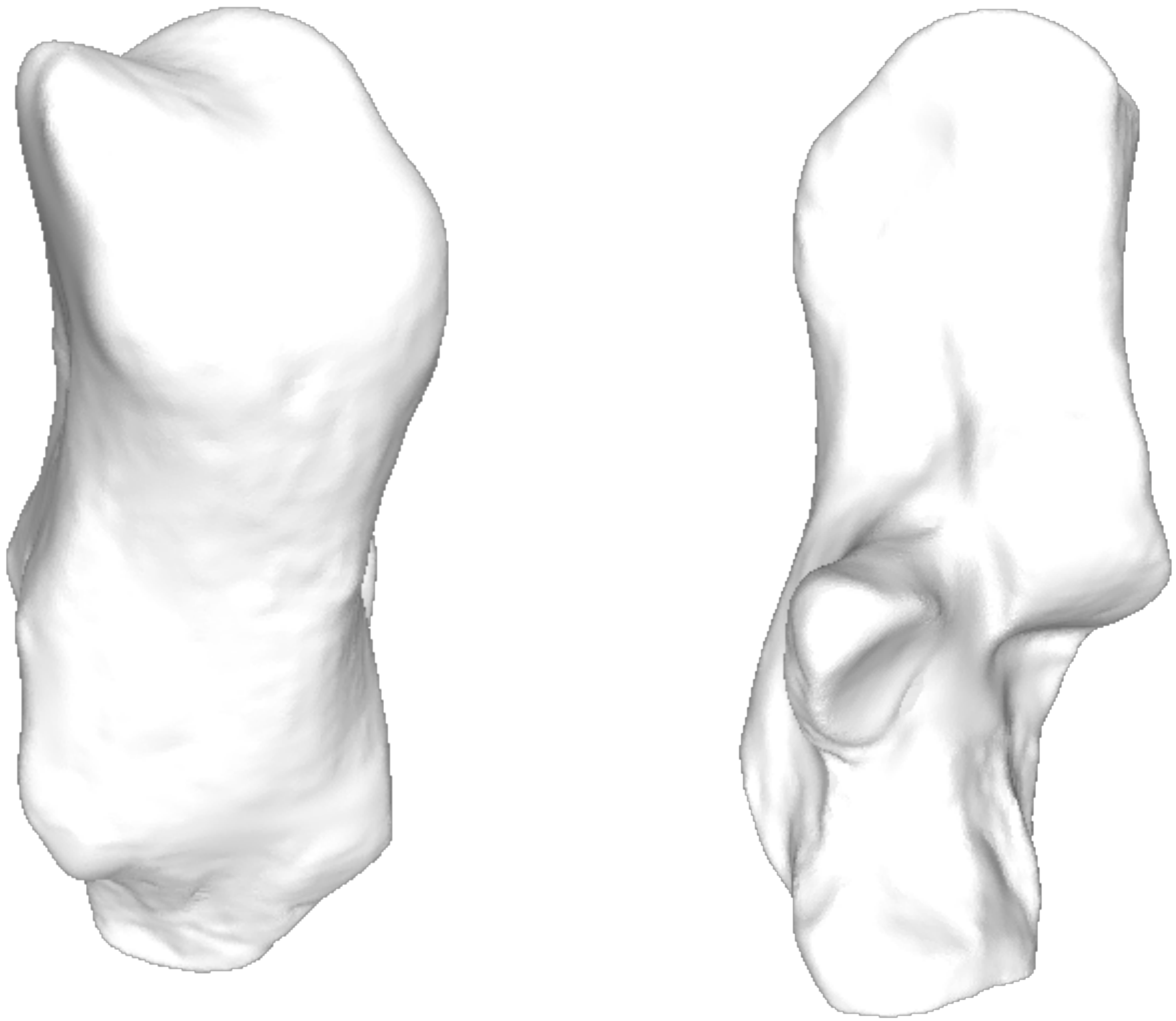
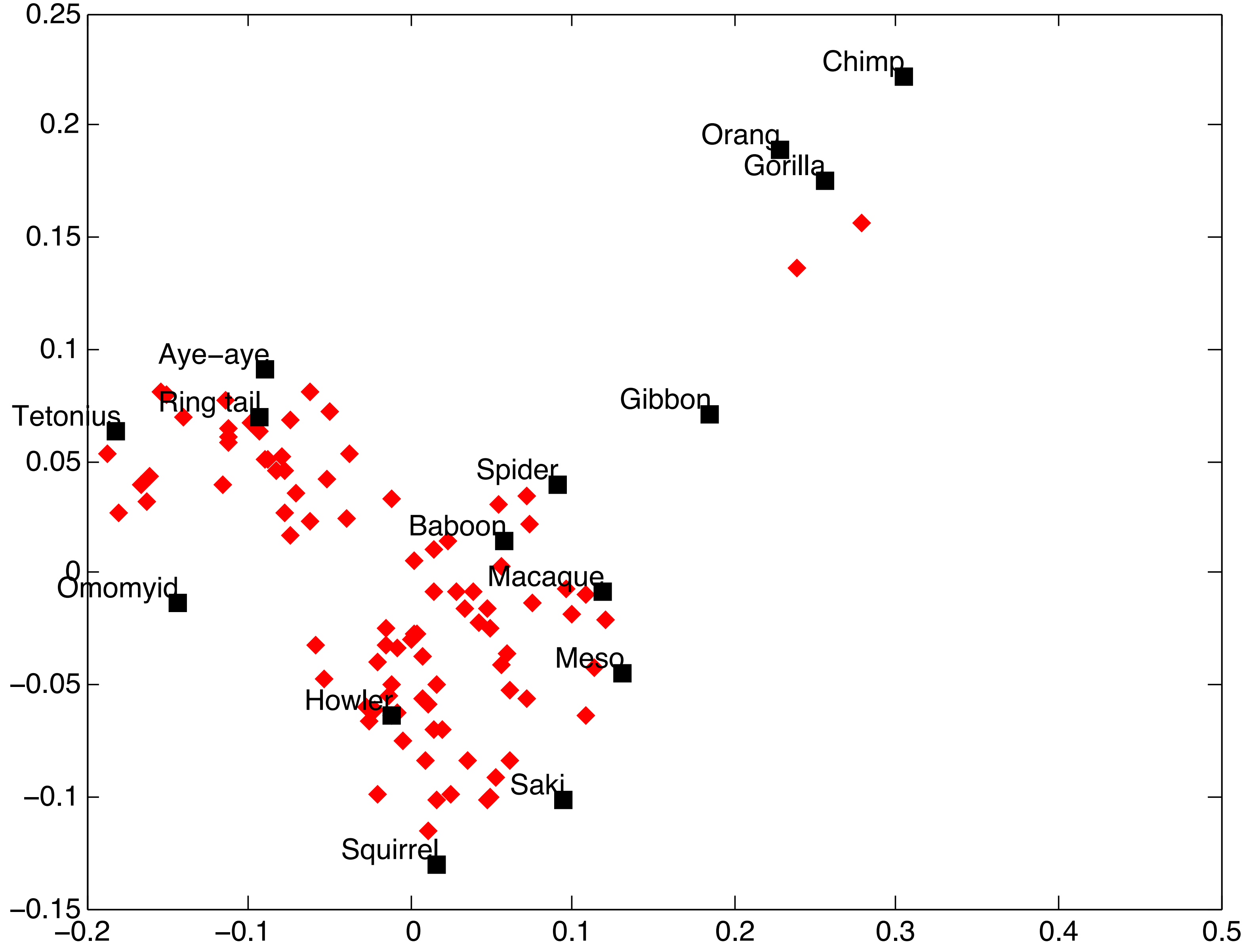
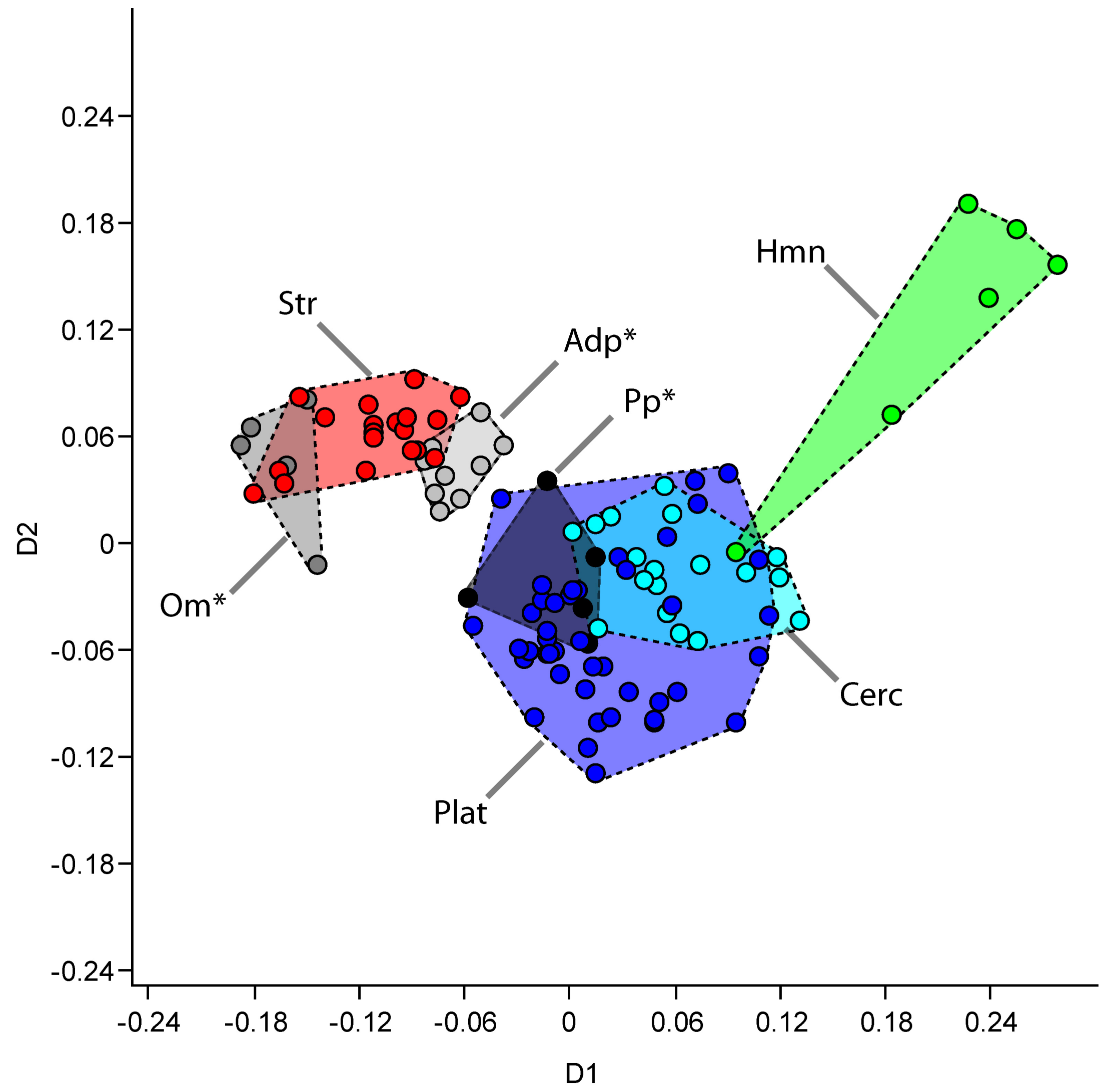


Figure: Images of a calcaneus from two different angles.

106 primates



Primate calcanei

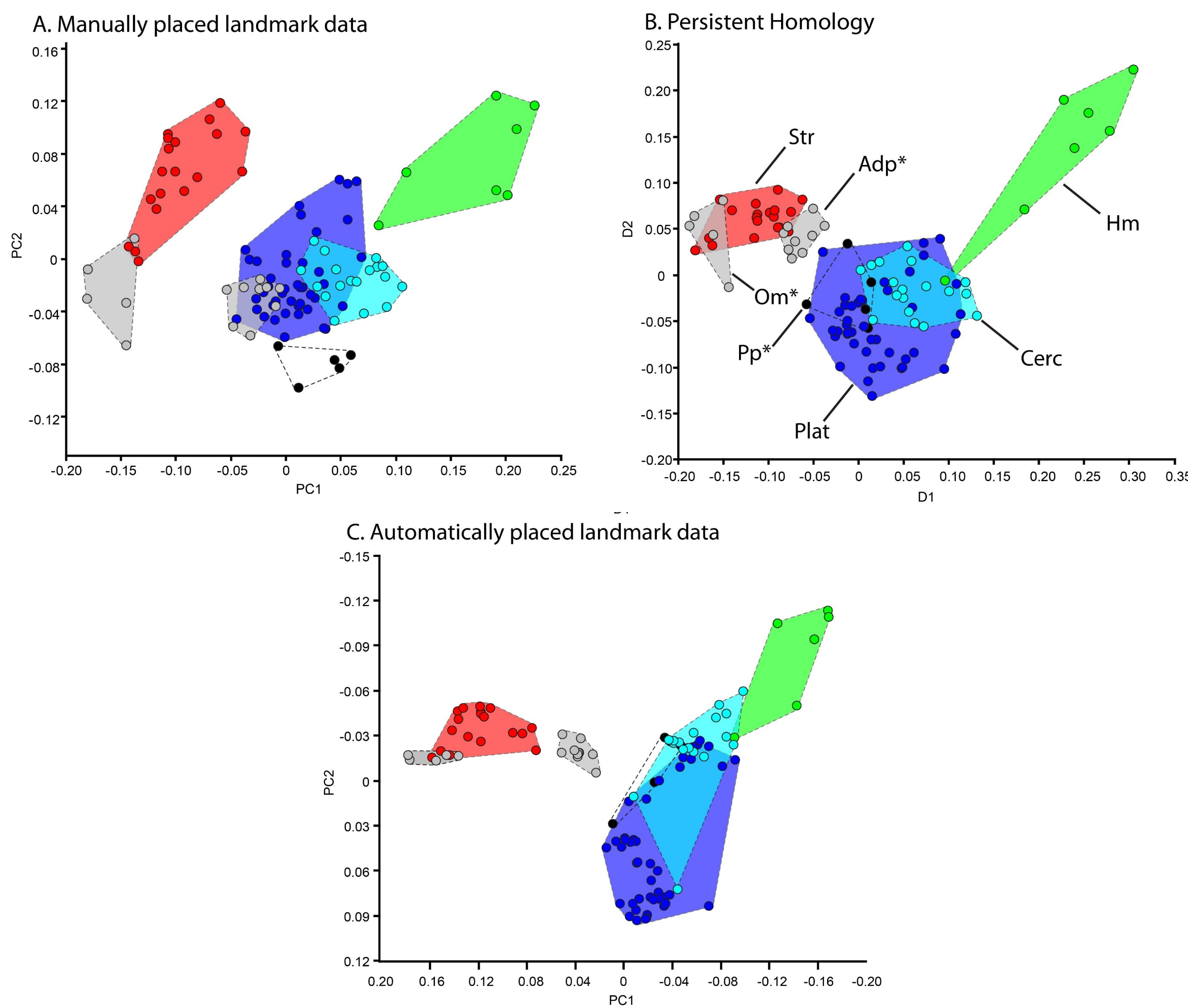


Phylogenetic groups of primate calcanei with 67 genera. Asterisks indicate groups of extinct taxa. Abbreviations: Str, Strepsirrhines; Plat, platyrrhines; Cerc, Cercopithecoids; Om, Omomyiforms; Adp, Adapiforms; Pp, parapithecids; Hmn, Hominoids.

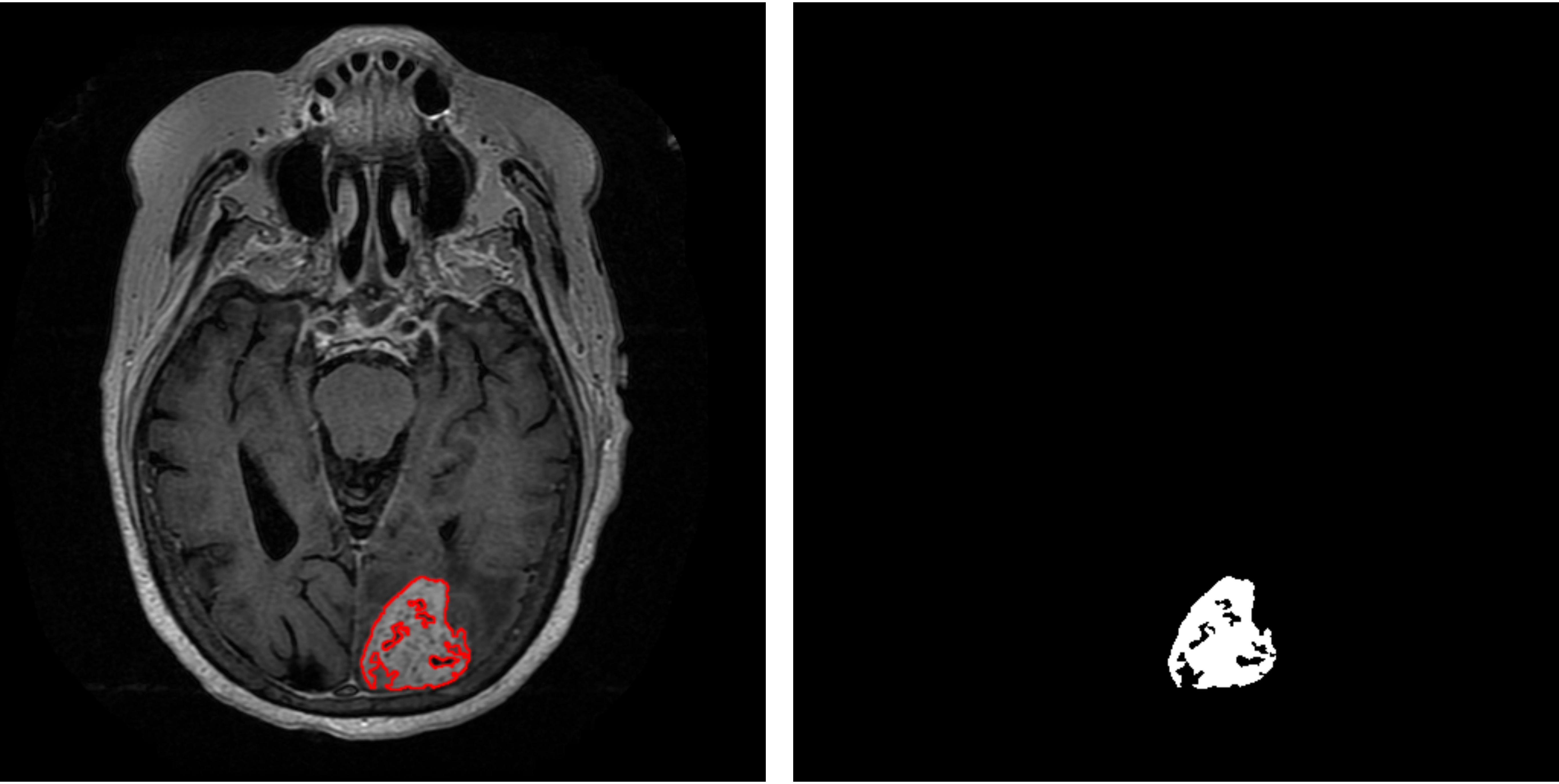
Comment from Doug

”In at least one way the method matched shapes with family groups better than any of the other previous methods... it linked a Hylobates specimen with the the other ape specimens (pan, gorilla, pongo, and oreopithecus). Previous both hylobatids (which ARE apes) always ended up closest to some Alouatta specimens.”

Comparing methods



Glioblastoma and radiogenomics



The data

92 patients with matched gene expression and MRI data from the TCGA.

Gene expression: $p_g = 9215$
Morphometric features: $p_m = 212$
Volumetric features: $p_v = 5$
Topological features: $p_s = 7200$

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Response:
Disease Free Survival (DFS): The period after a successful treatment during which there are no signs or symptoms of the cancer that was treated.
Overall Survival (OS): The entire period after the start of treatment during which the cancer patient is still alive.

The question I

Which of the following best explains variation in the clinical trait:
Gene expression: $p_g = 9215$
Morphometric features: $p_m = 212$
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Using shapes in regression models.

The model

Consider the following kernel model

$$f(\mathbf{F}) = \sum_{i=1}^{n} \alpha_i \, k(\mathbf{F}, \mathbf{F}_i) \, .$$

Can use standard functional data analysis. The same as used in genomic selection.

Results

		Disease Free Survival (DFS)			Overall Survival (OS)		
Covariance Function(s)	Data Type	R^2	Optimal%	$\widehat{\theta}$	R^2	Optimal%	$\widehat{\theta}$
Linear Kernel	Gene Expression	0.090 (0.010)	16.2%	—	0.065 (0.03)	13.5%	—
	Morphometrics	0.135 (0.010)	26.7%	—	**0.133 (0.05)**	**34.5%**	—
	Geometrics	0.126 (0.01)	20.9%	—	0.111 (0.04)	28.3%	—
	SECT	**0.199 (0.01)**	**36.2%**	—	0.101 (0.04)	23.7%	—
Gaussian Kernel	Gene Expression	0.121 (0.05)	22.2%	4.3	0.076 (0.03)	21.9%	10.0
	Morphometrics	0.084 (0.03)	12.8%	0.1	0.038 (0.03)	8.0%	4.0
	Geometrics	0.154 (0.06)	25.2%	5.2	0.085 (0.04)	22.1%	5.0
	SECT	**0.235 (0.08)**	**39.8%**	0.6	**0.171 (0.06)**	**48.0%**	4.2
Cauchy Kernel	Gene Expression	0.069 (0.03)	22.7%	6.4	0.048 (0.02)	16.8%	10.0
	Morphometrics	0.036 (0.02)	10.0%	1.2	0.071 (0.03)	25.6%	4.5
	Geometrics	0.062 (0.03)	14.6%	0.2	0.050 (0.02)	15.9%	3.5
	SECT	**0.212 (0.07)**	**52.7%**	0.6	**0.113 (0.04)**	**41.7%**	5.5

Subimage selection: question II

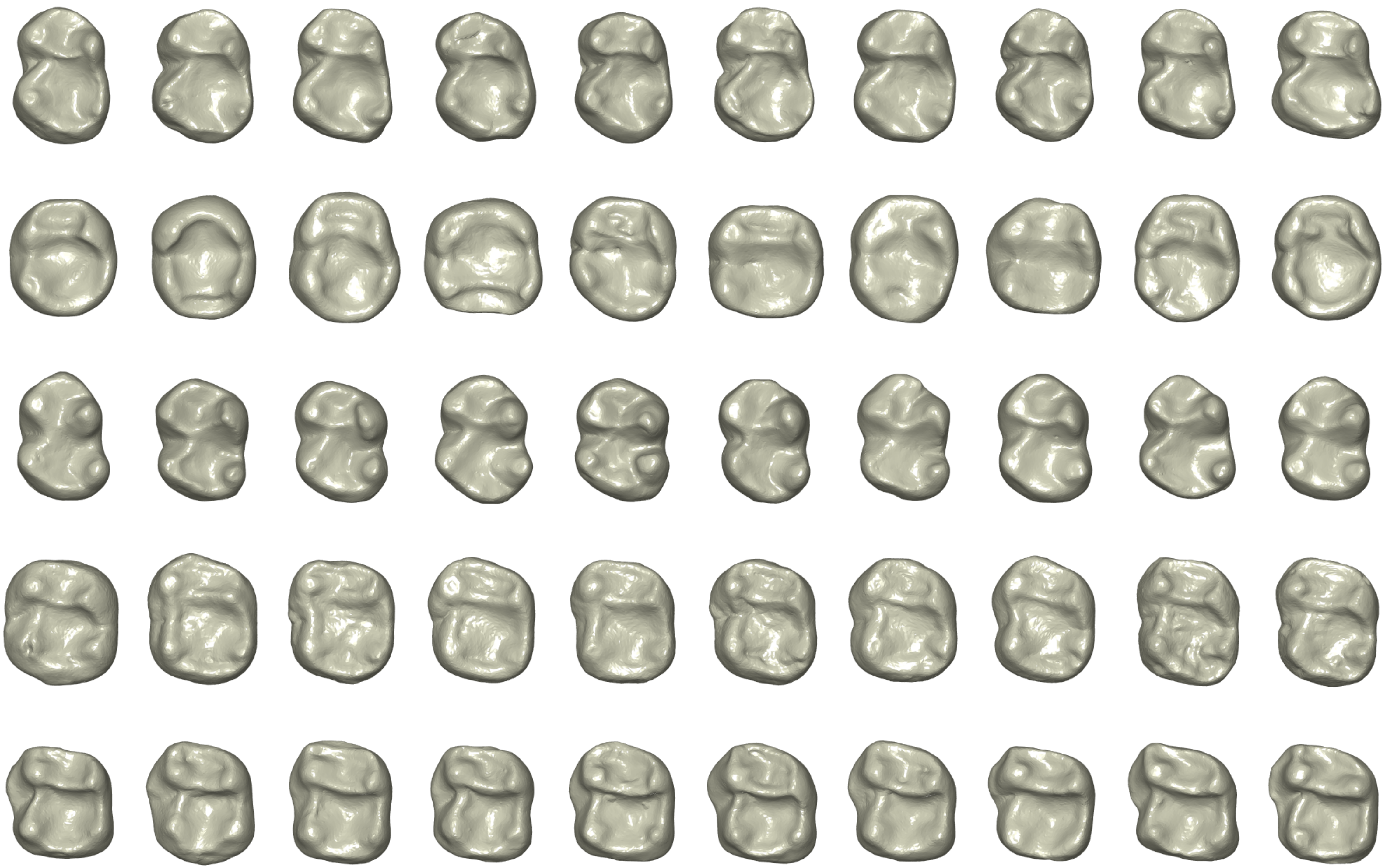
What parts of the shape are most associated to variation in trait ?

Subimage selection: question II

What parts of the shape are most associated to variation in trait ?

This is a variable selection problem in the regression framework.

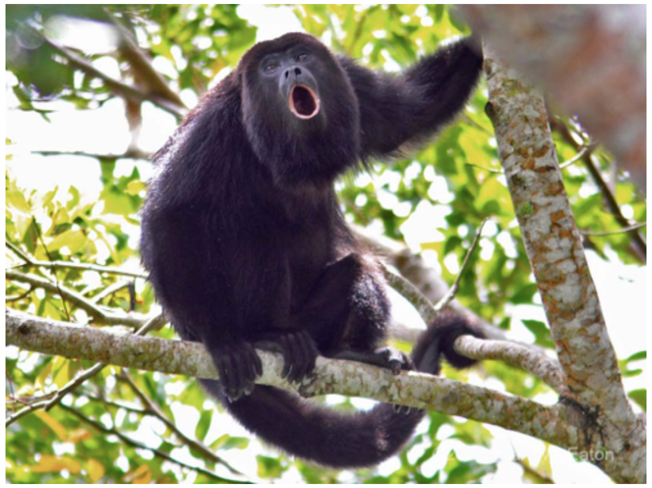
50 molars from 5 primate genera



5 primate genera

Spider monkey

Howler Monkey

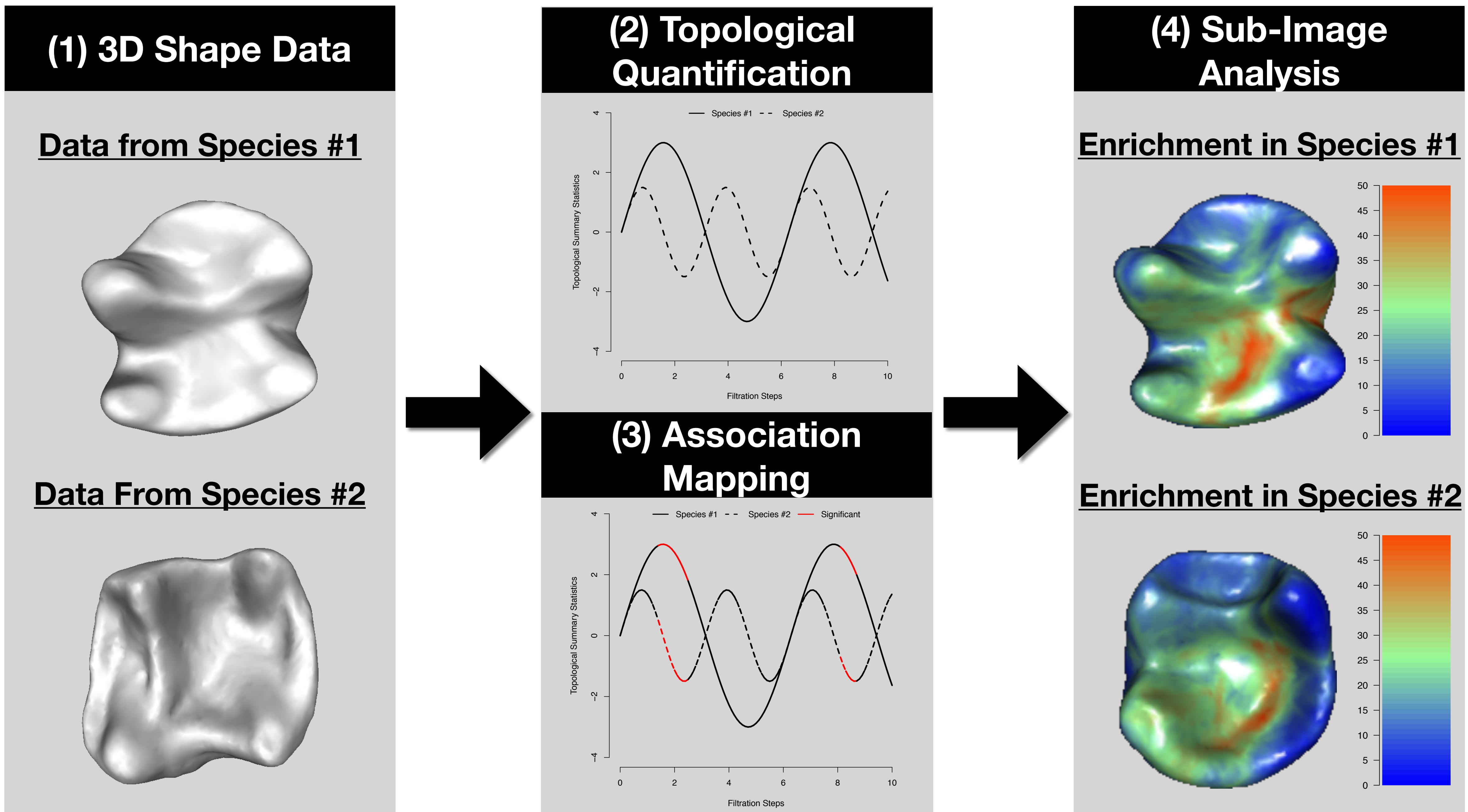


Squirrel Monkey

Black handed spider monkey

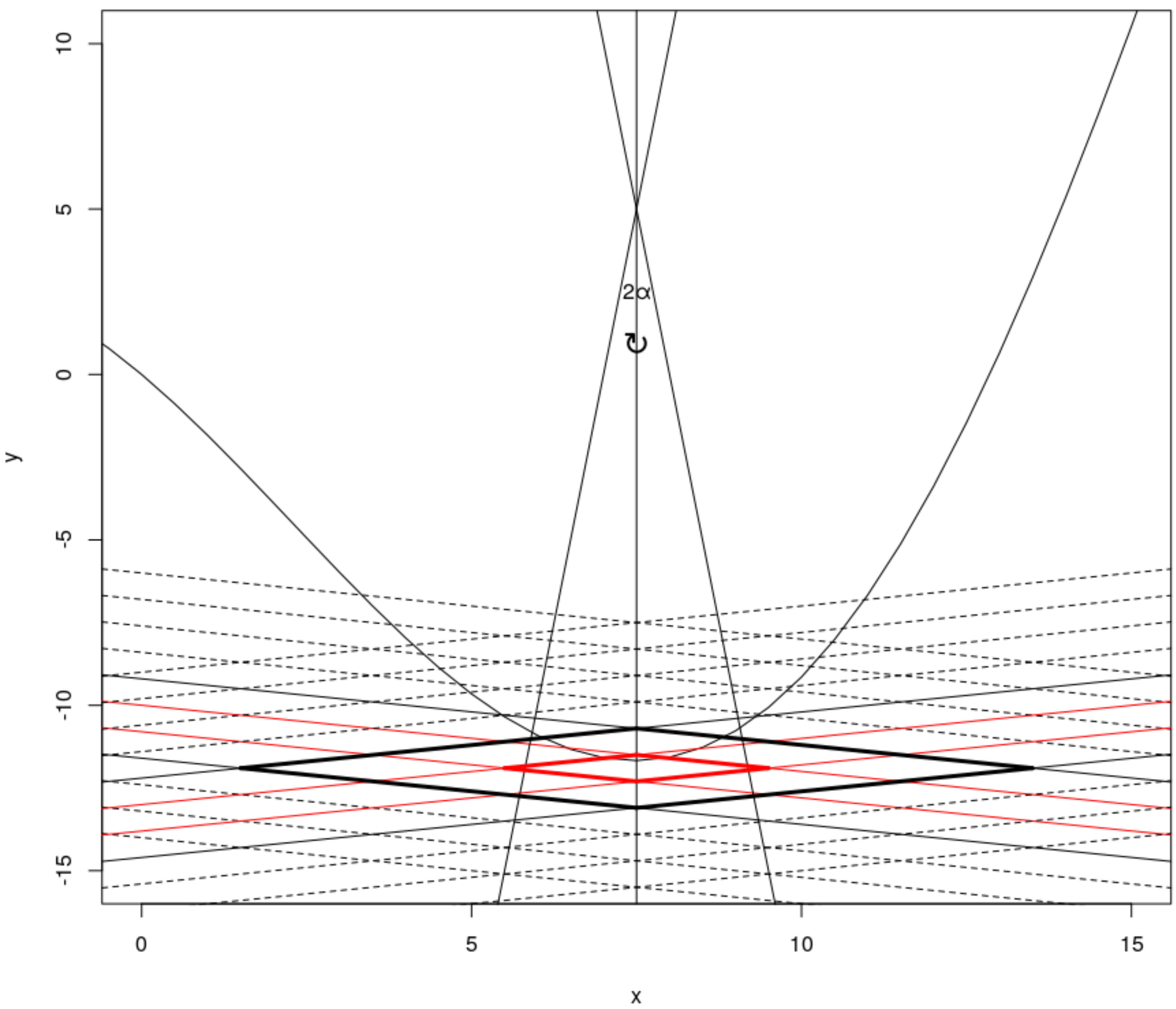
Titi monkey

Subimage selection



Henry Kirveslahti, Bruce Wang, Tim Sudijono

Ray tracing



Open questions and problems

(1) Localized transforms: The PHT and ECT can be generalized as Euler integration

$$\int_X h \, d\chi, \quad h \text{ is a (localized) basis function.}$$

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(6) Generalization to graphs and networks.

Evolution of cooperation in mammals

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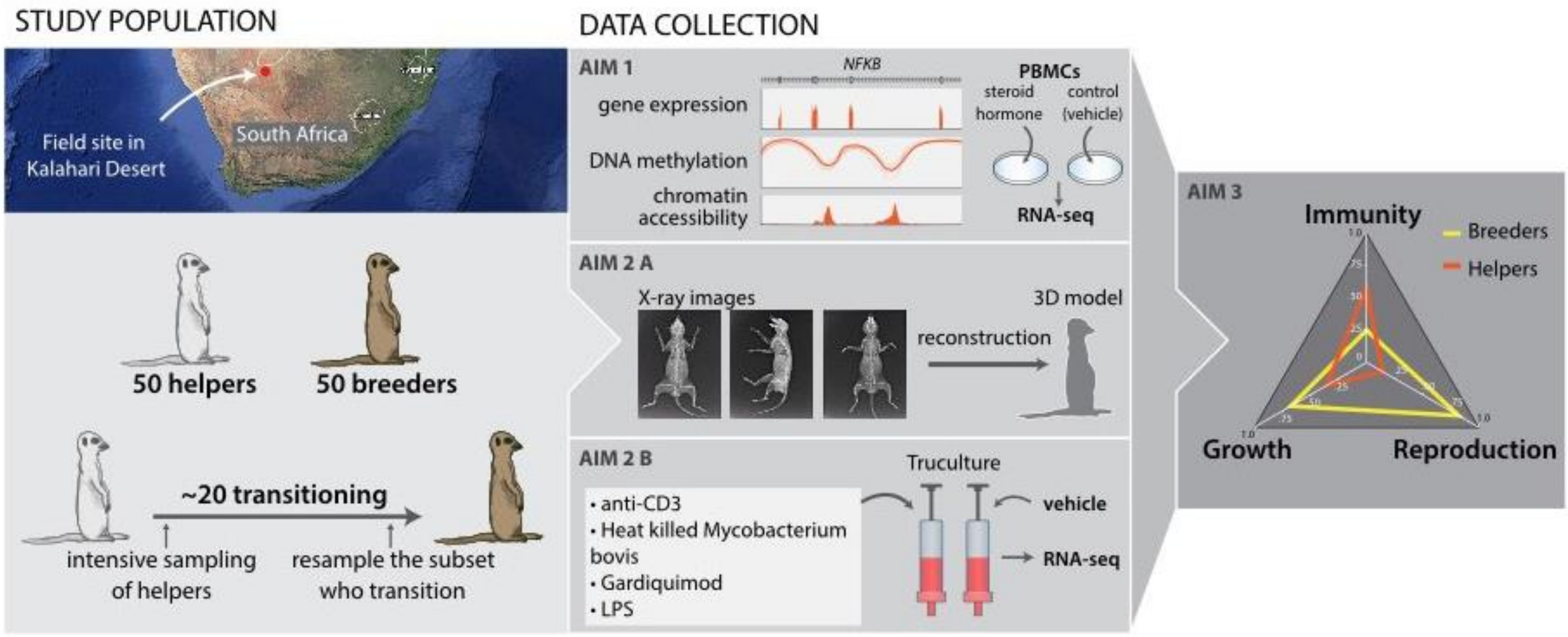

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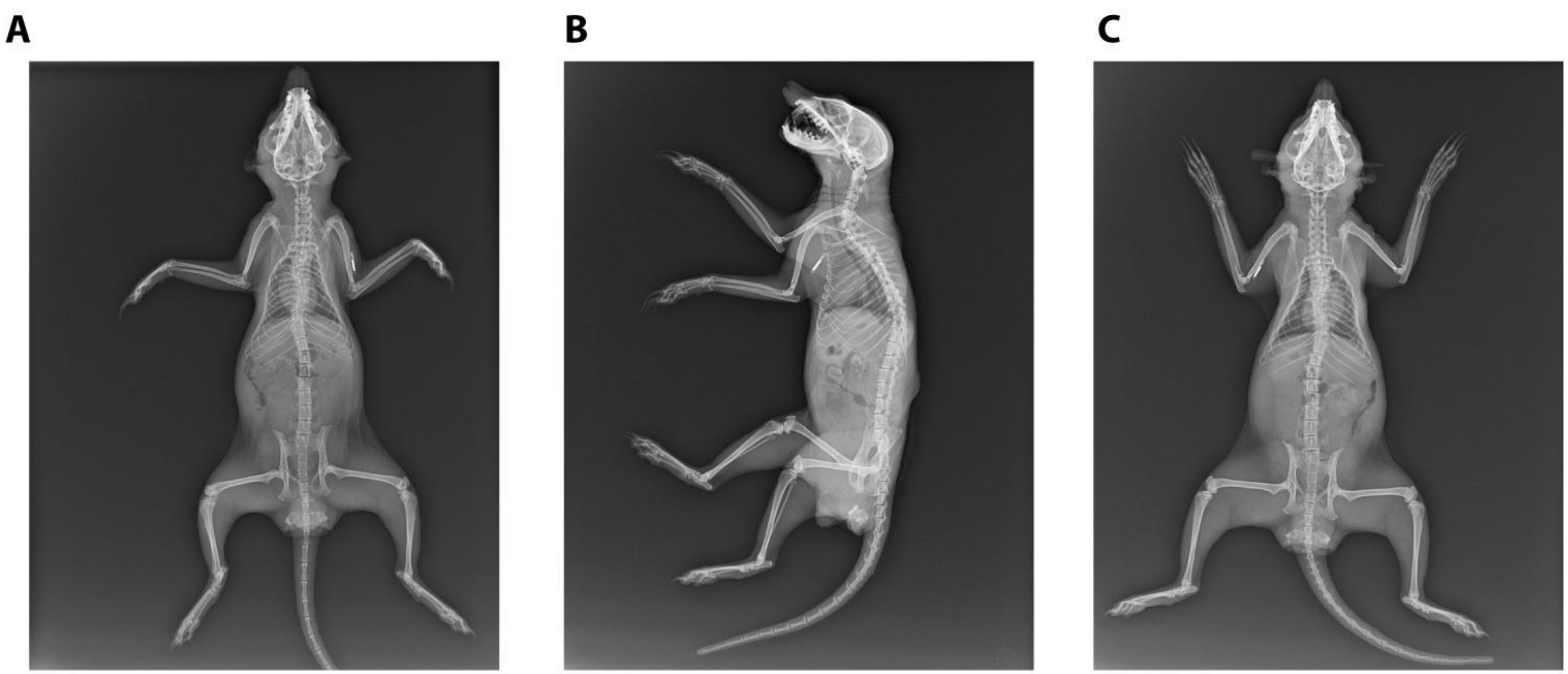

Collaborators

In this talk:

Integral geometry: K Turner (ANU), J. Curry (Albany), D. Boyer (Duke)

Regression: L. Crawford (Brown) , A. Monod, R. Rabadán, A. Chen (Columbia)

Variable selection: H. Kirveslahti (Duke), L. Crawford, T. Sudijono, B. Wang (Brown)

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Thank You
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Vinaka
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спасибо
감사합니다
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ارك شكرا
Manana
Dankon
Mauruuru
Biyan
Diolch i Chi
Terima Kasih
Matondo
Taiku
Tack
Dank Je
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Mochchakkeram
Gracias
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Khap
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Ua Tsaug Rau Koj
Grazas
Kia Ora
Obrigado
Děkuji
Nirringrazzjak
Di Ou Mèsi
Kop Khun
ありがとう
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Matur Nuwun
Rahmat
Hvala
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谢谢
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