Persistent homology for biology

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Outline

1. Data
2. Persistent homology
3. Ordinary persistence: one parameter
4. Multiple parameters: fruit fly wings
5. Tameness
6. History of persistent homology
7. Bar codes
8. Statistical analysis
9. Lessons on persistence
10. Future directions

What kinds of data?

Shapes

- 1D: curves (in $\mathbb{R}^2$ or $\mathbb{R}^3$, say)
- 2D: photographs
- 3D: MRI, DTI, SPECT, PET, CAT, integrated photo
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  - brain arteries
  - lung airways
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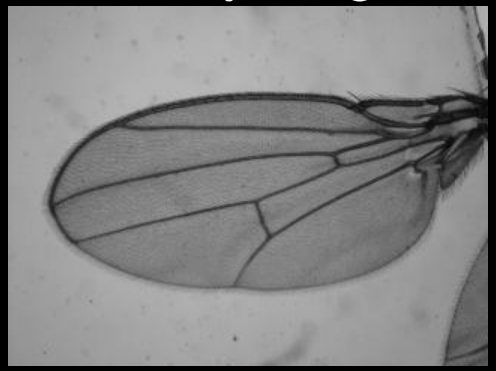
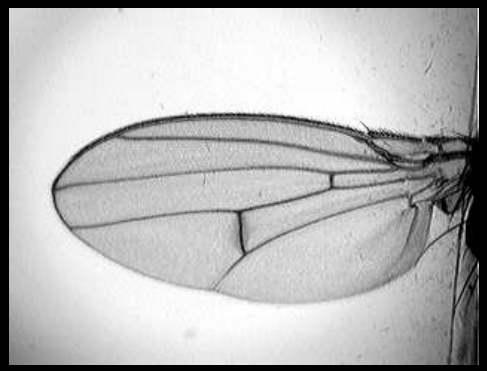
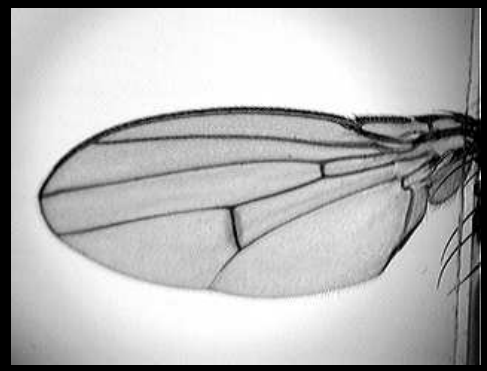
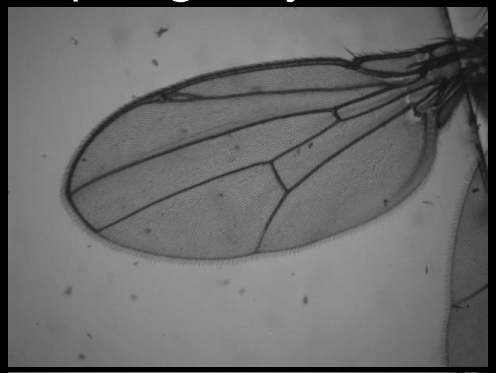
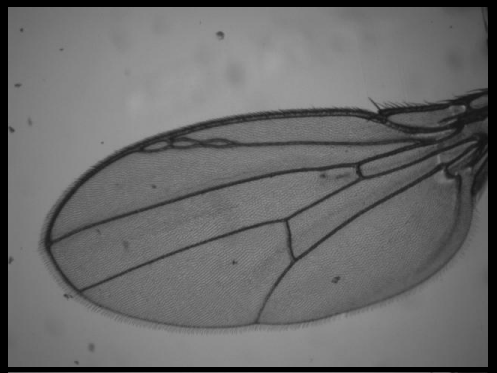
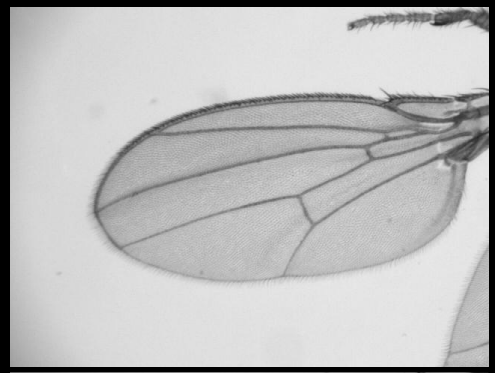
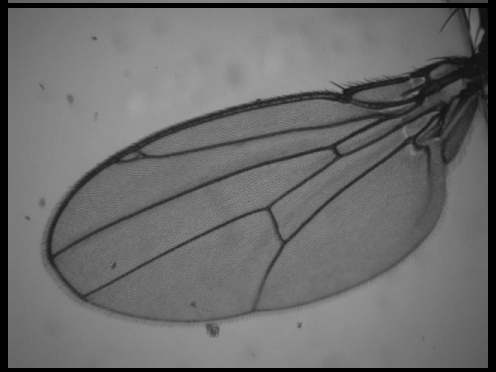
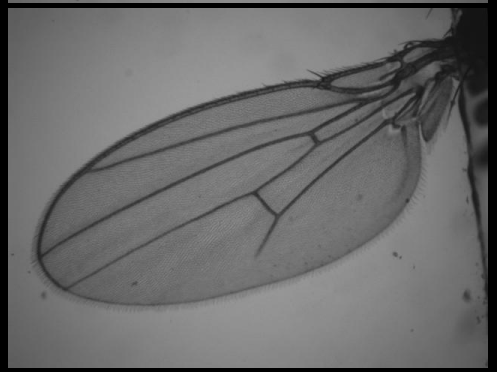
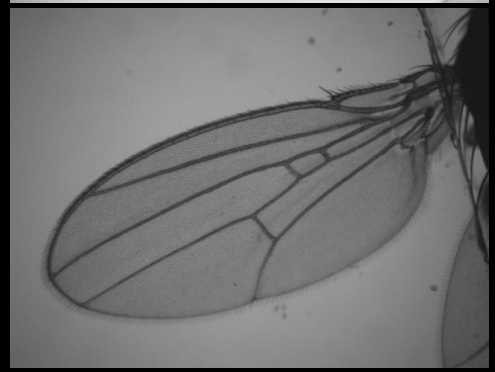
Fruit fly wings

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

Topologically abnormal veins:

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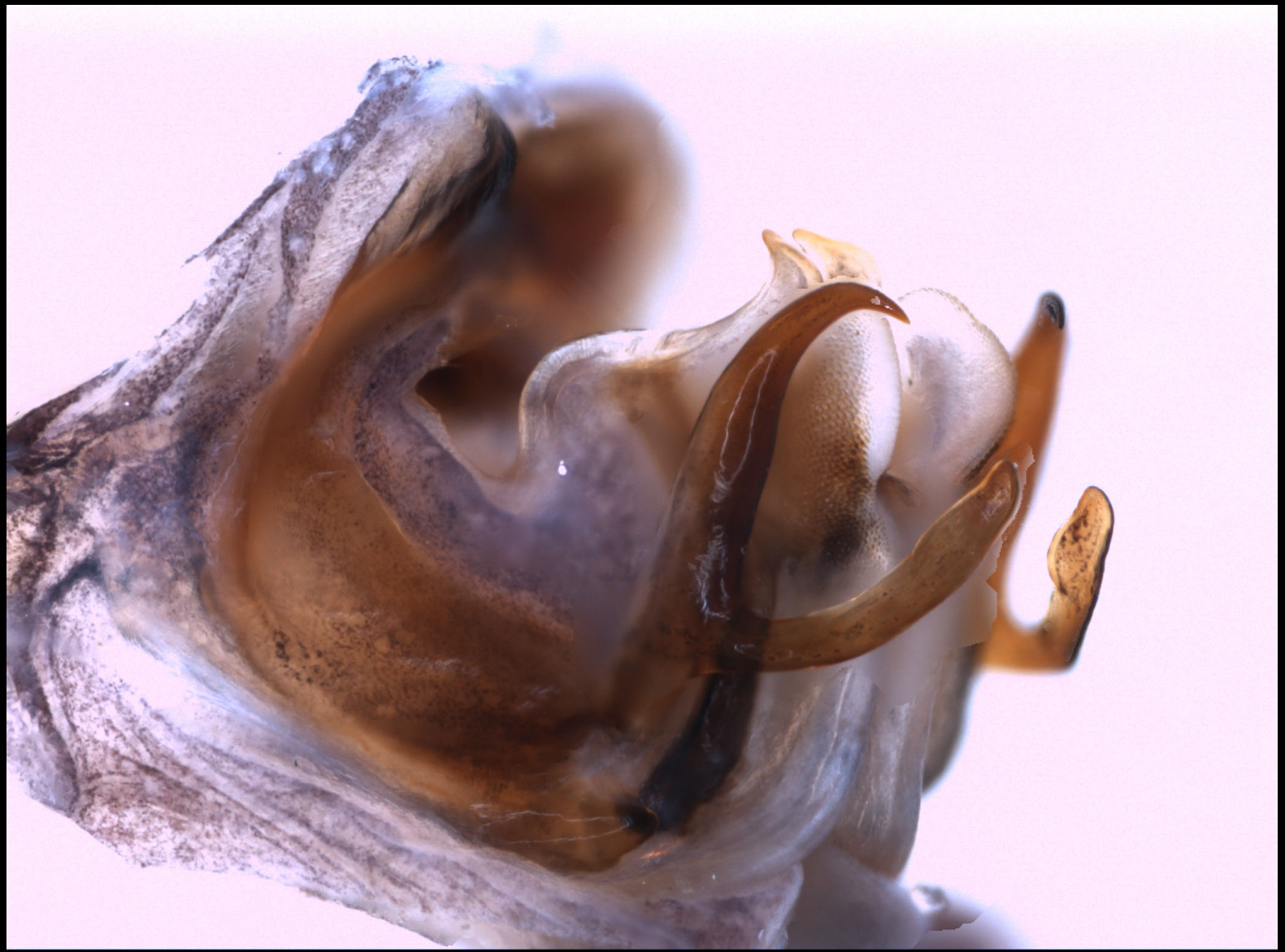

courtesy Elen Oneal

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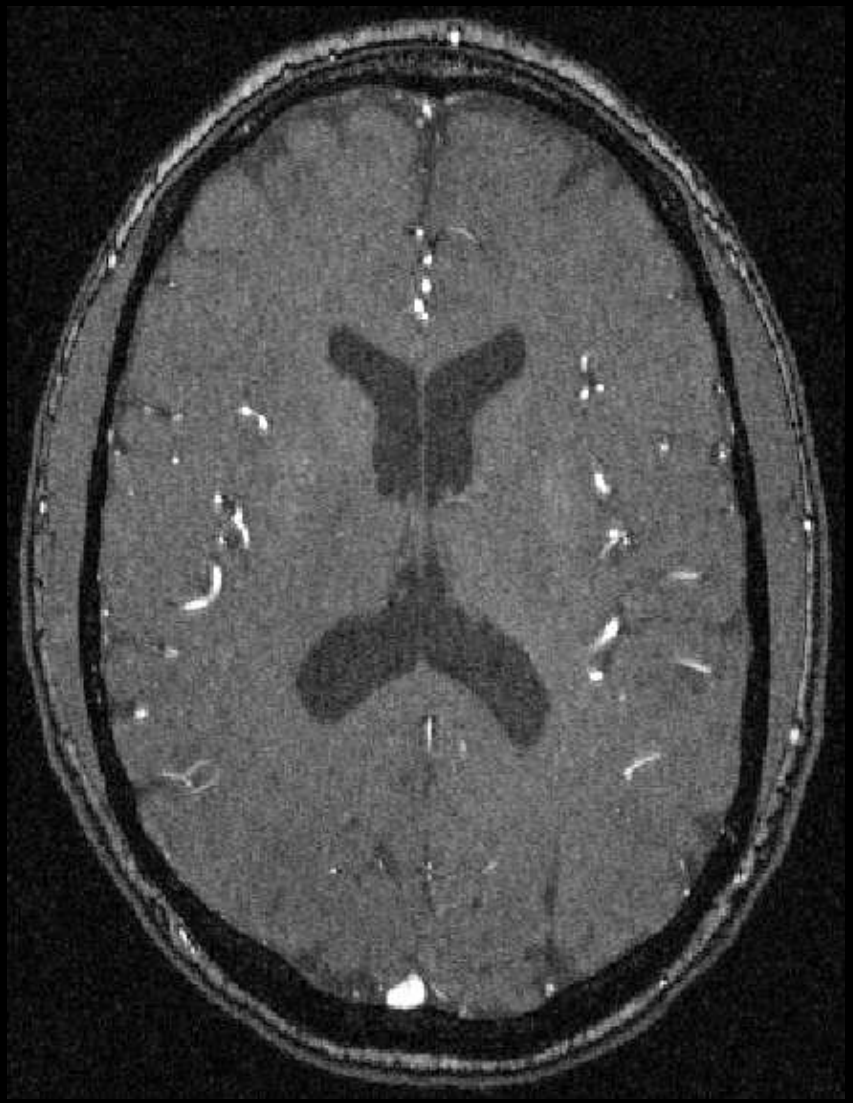

courtesy Elizabeth Bullitt, Dept. of Neurosurgery, UNC-CH

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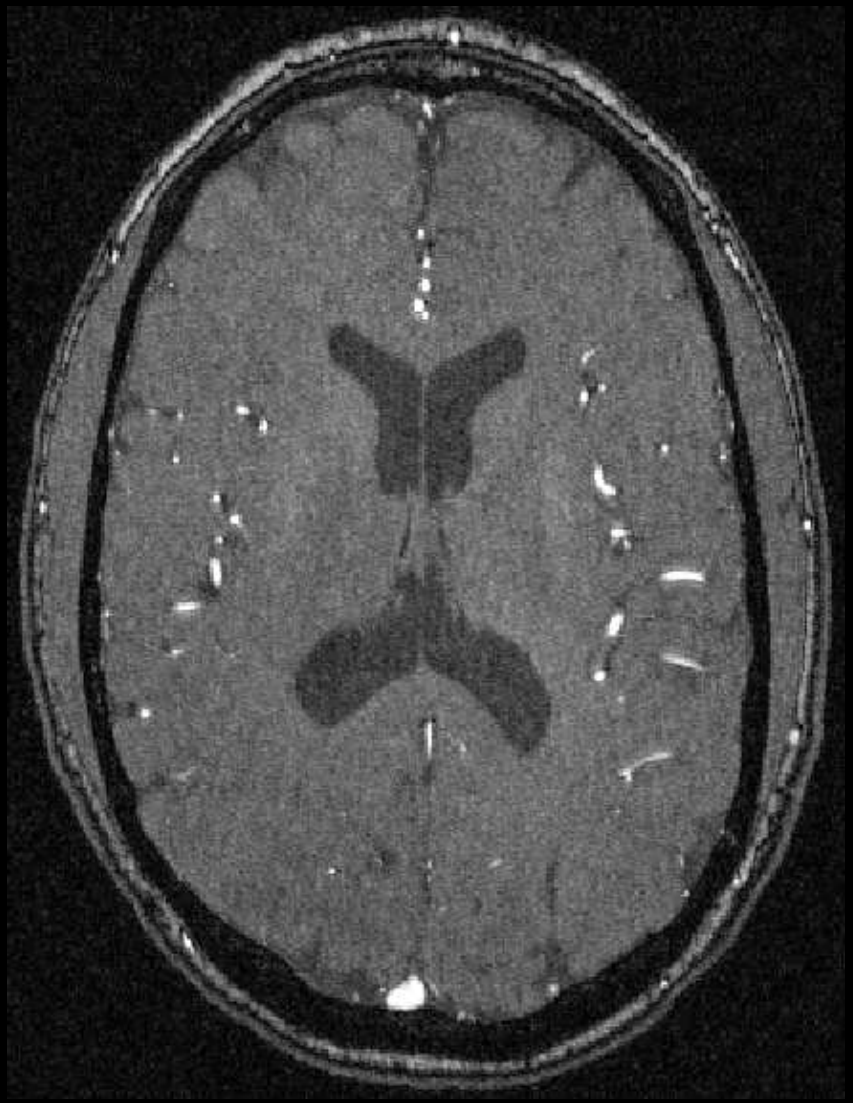

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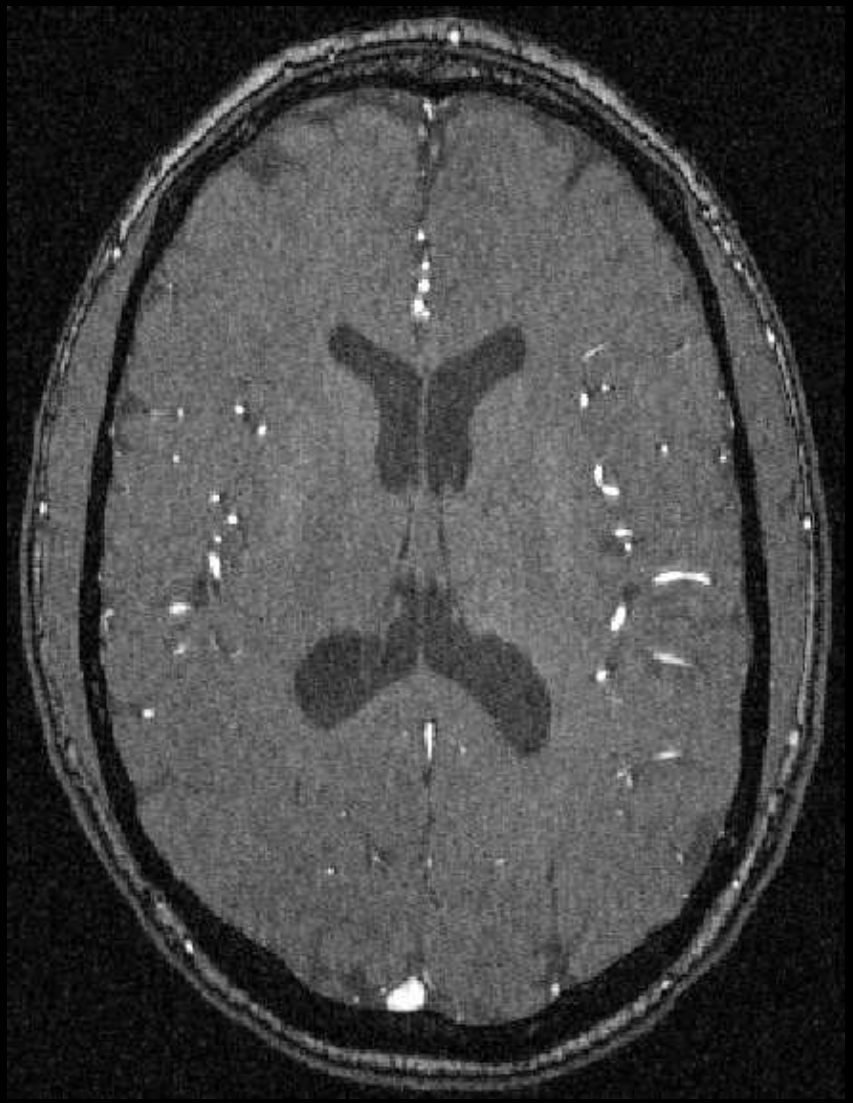

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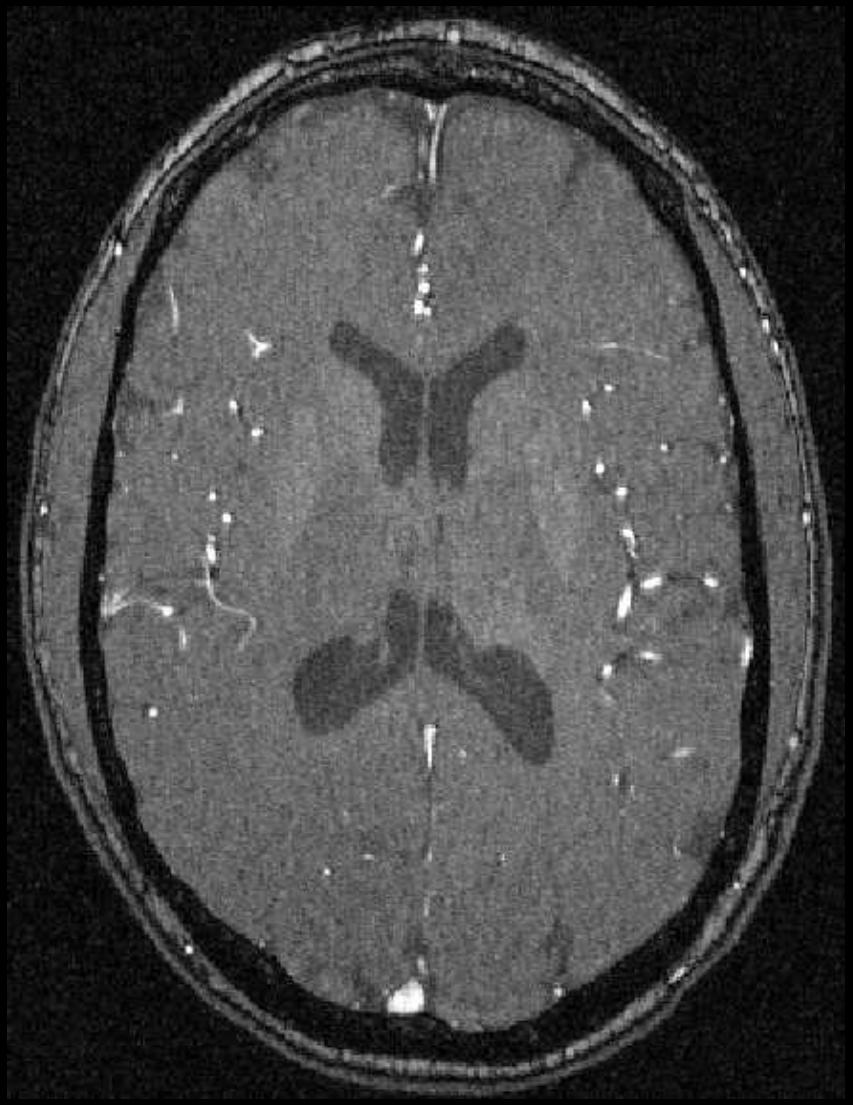

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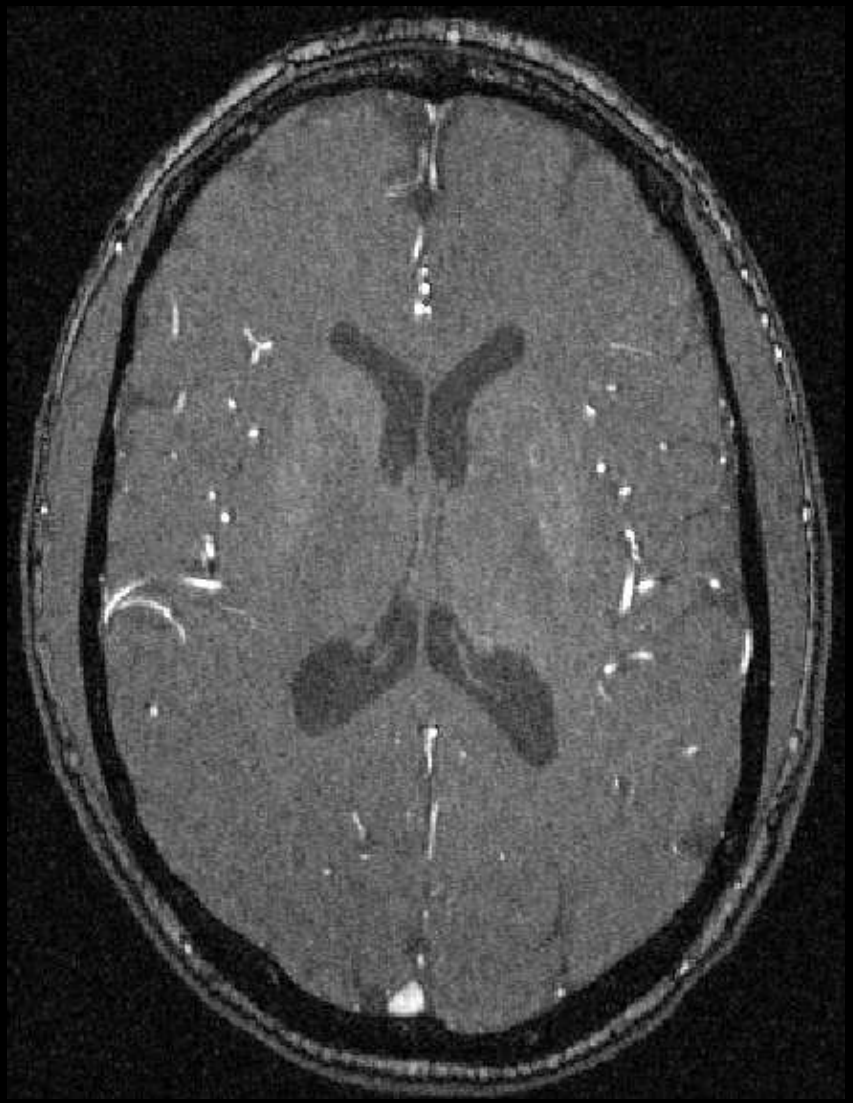

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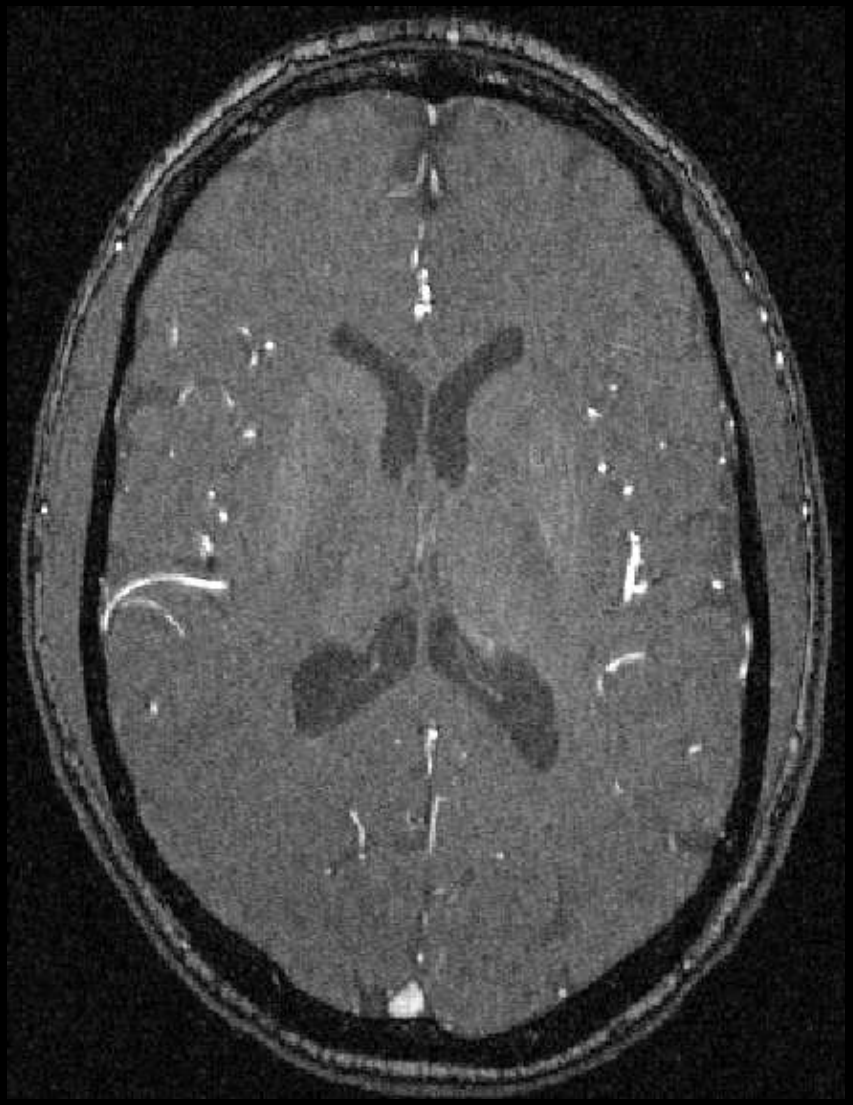

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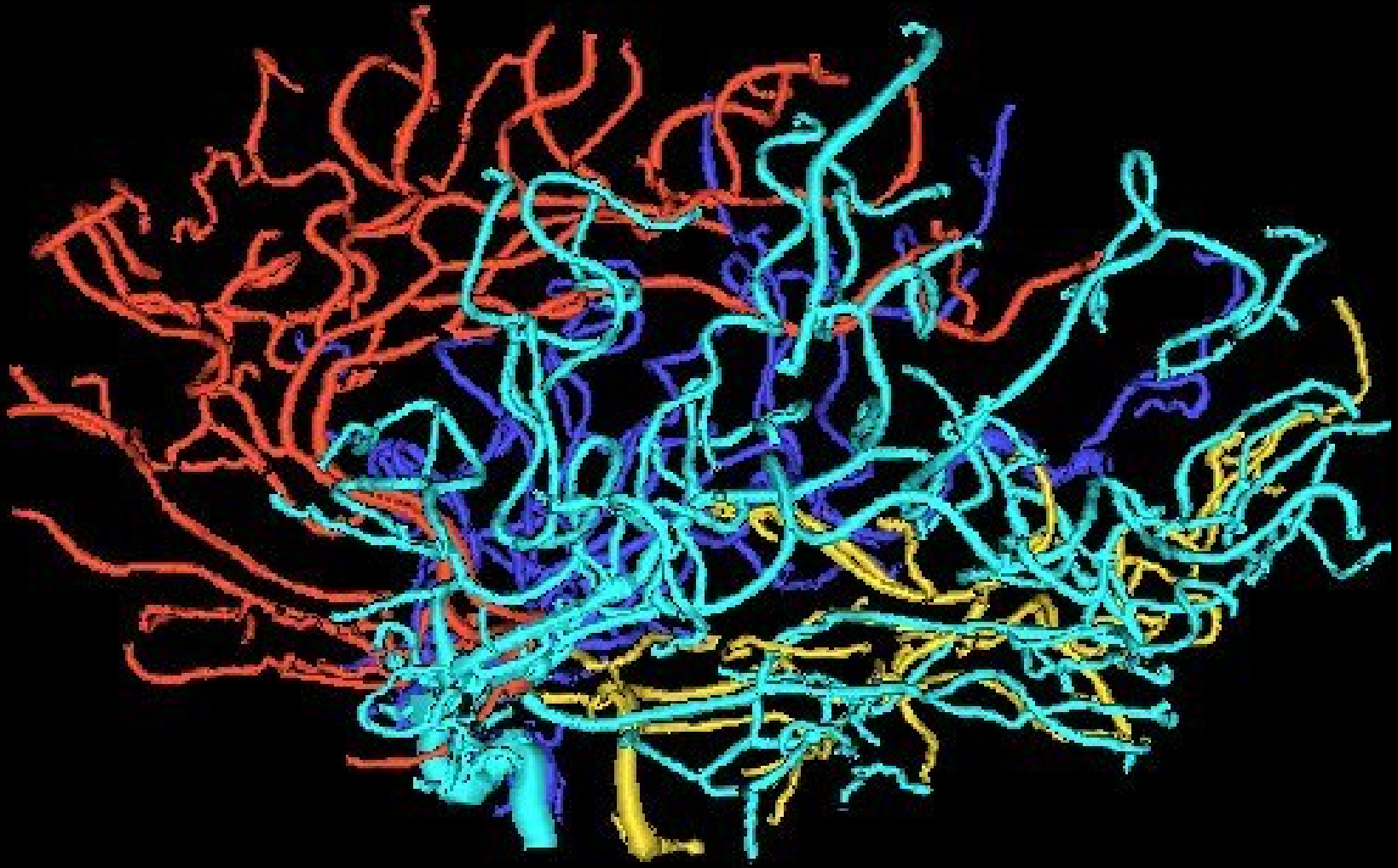
Brain arteries



[Bullitt and Aylward, 2002]

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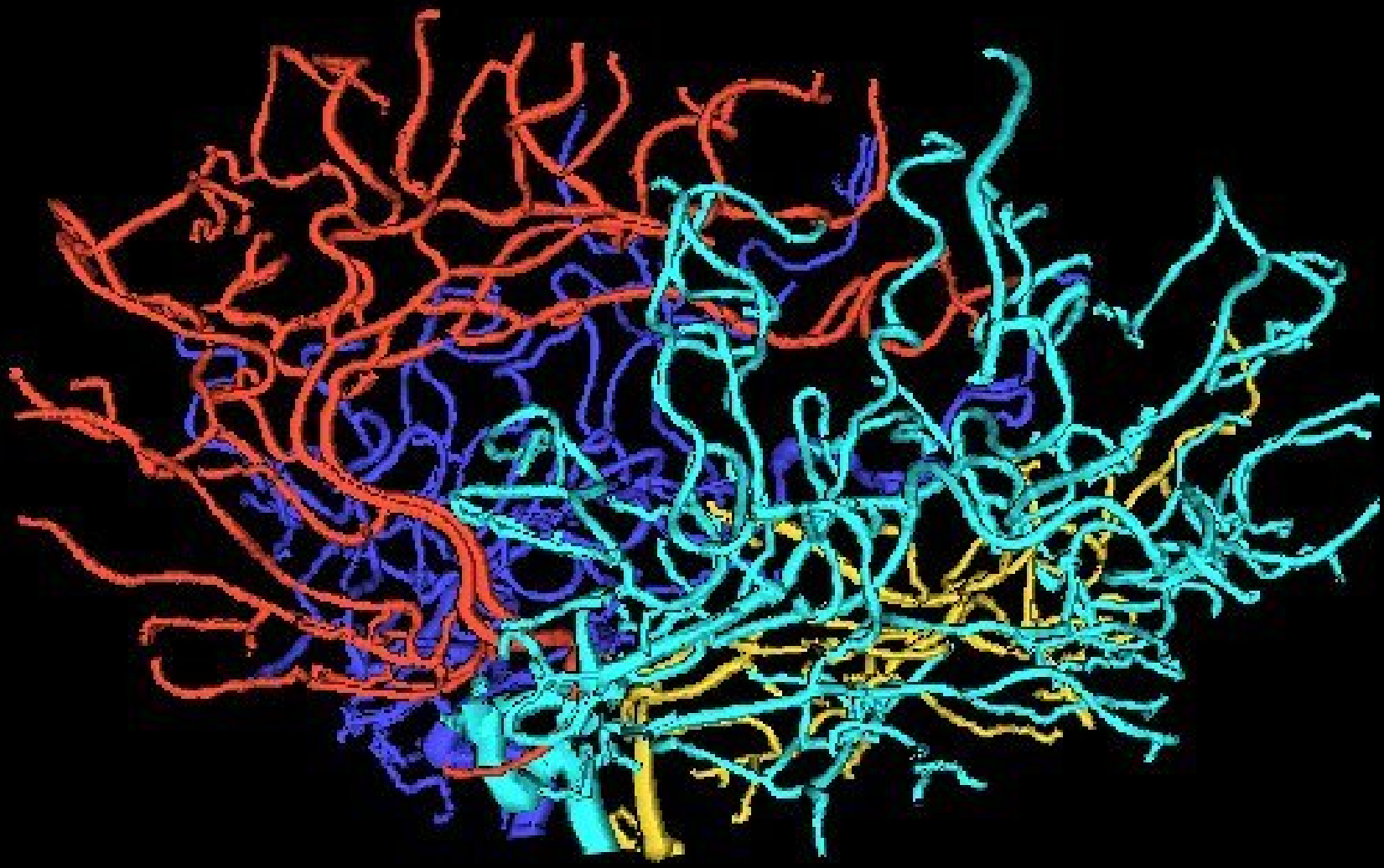

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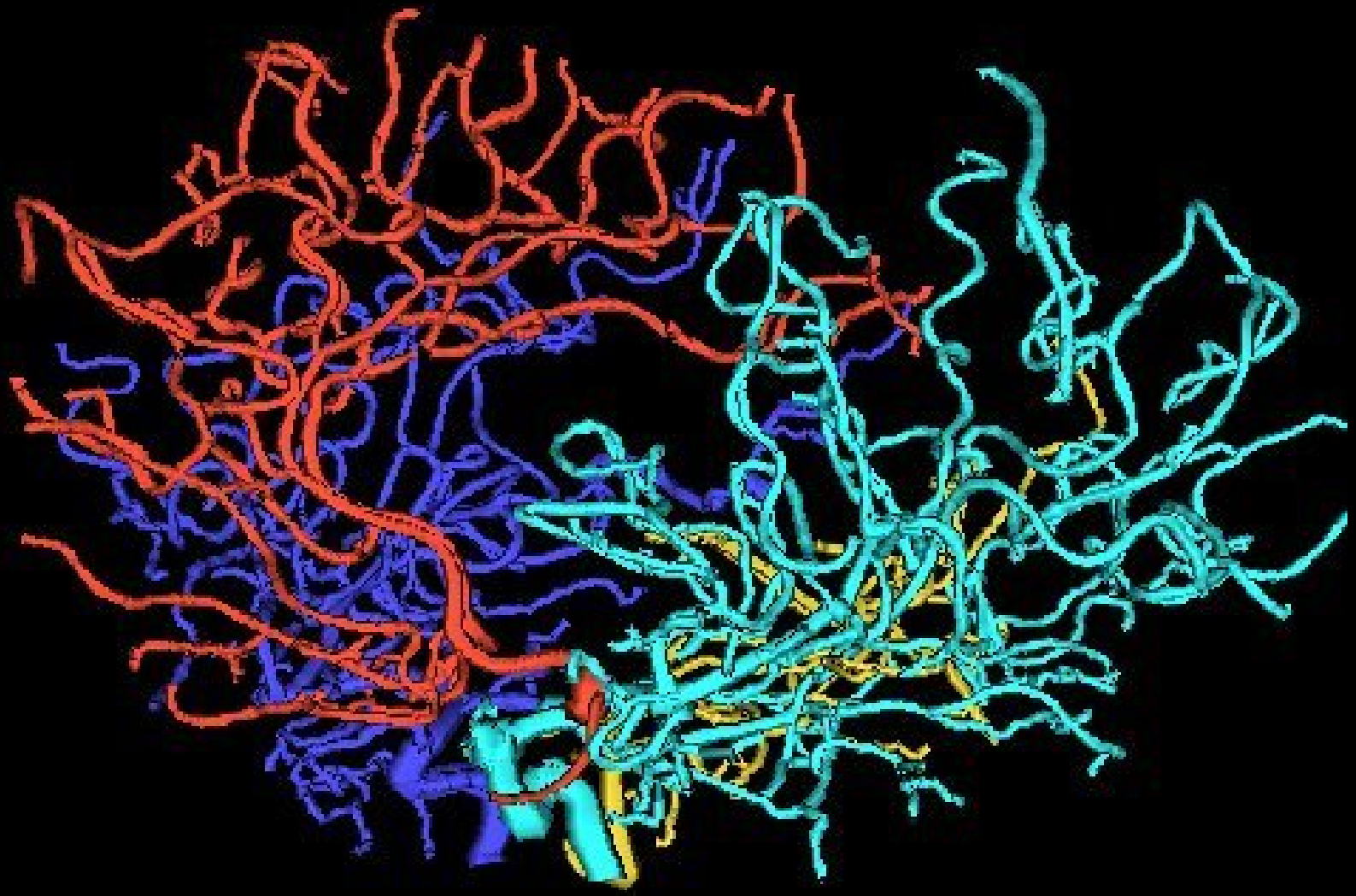

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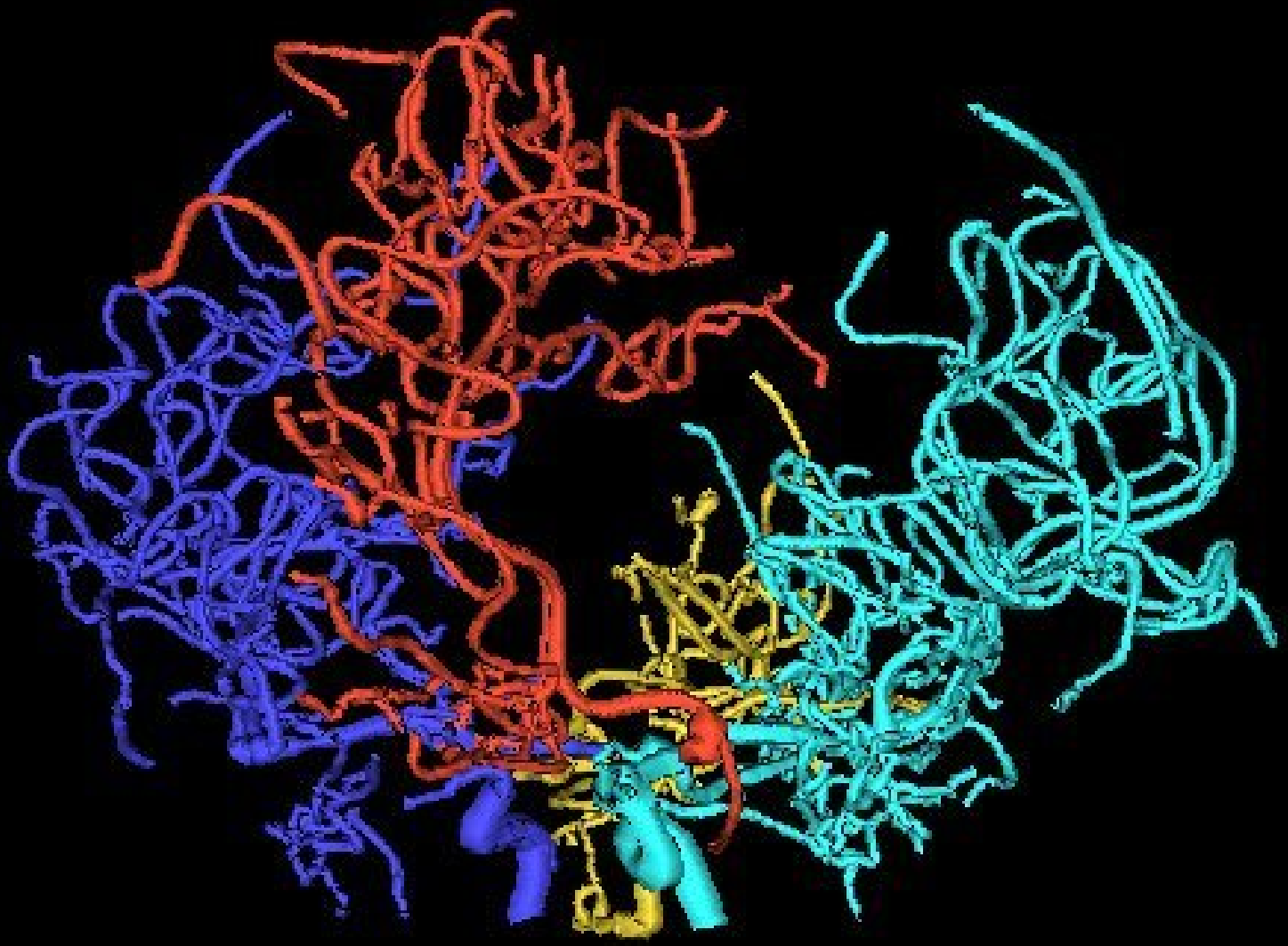

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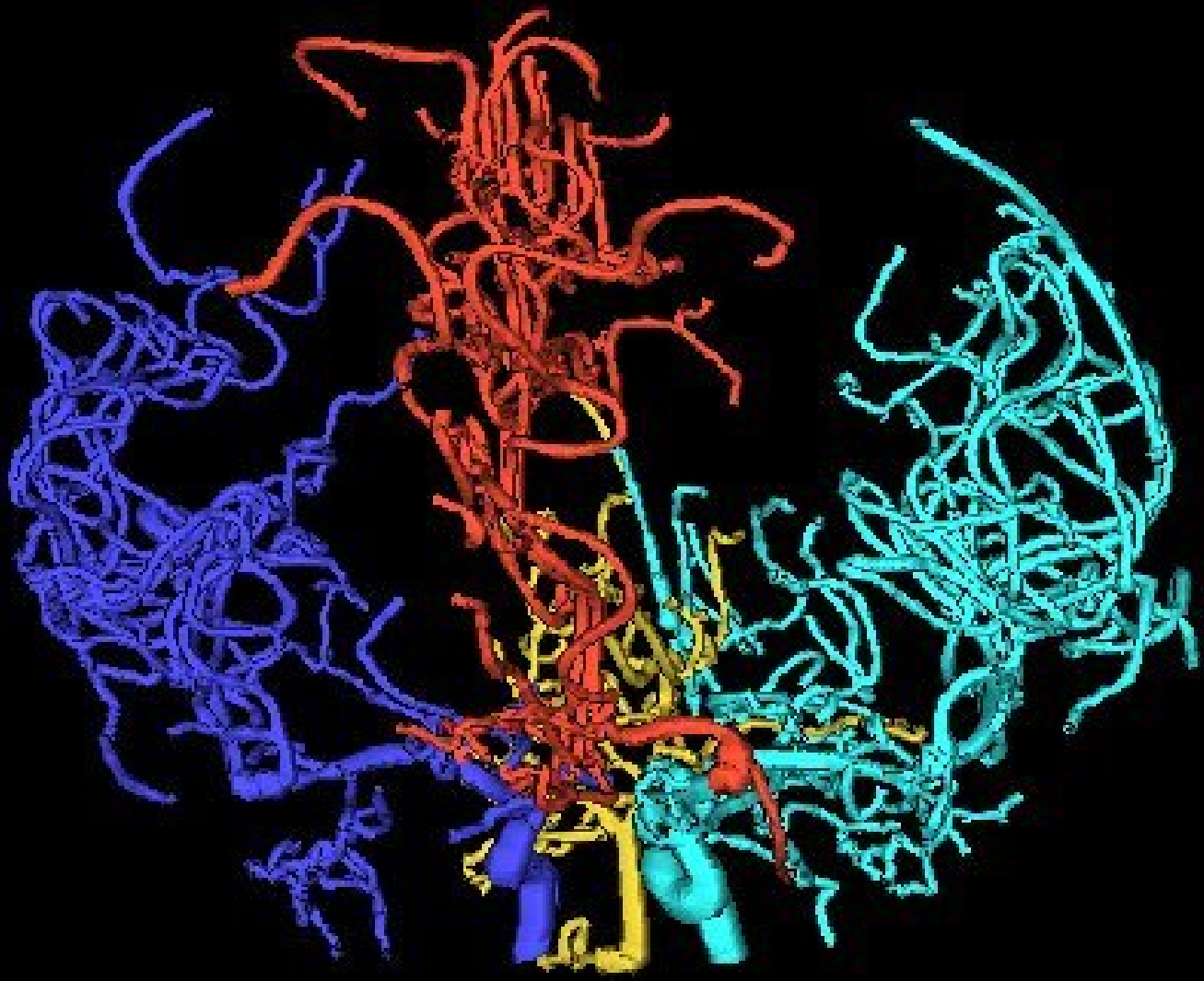

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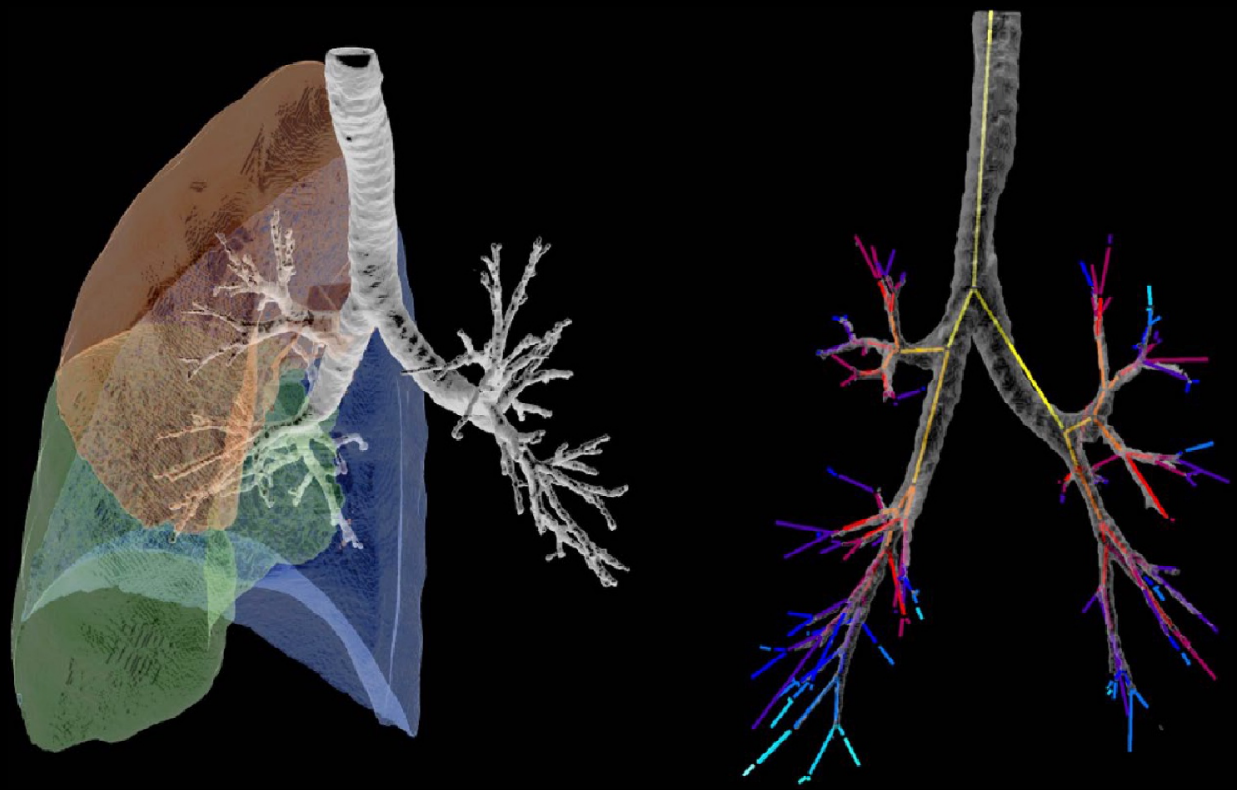
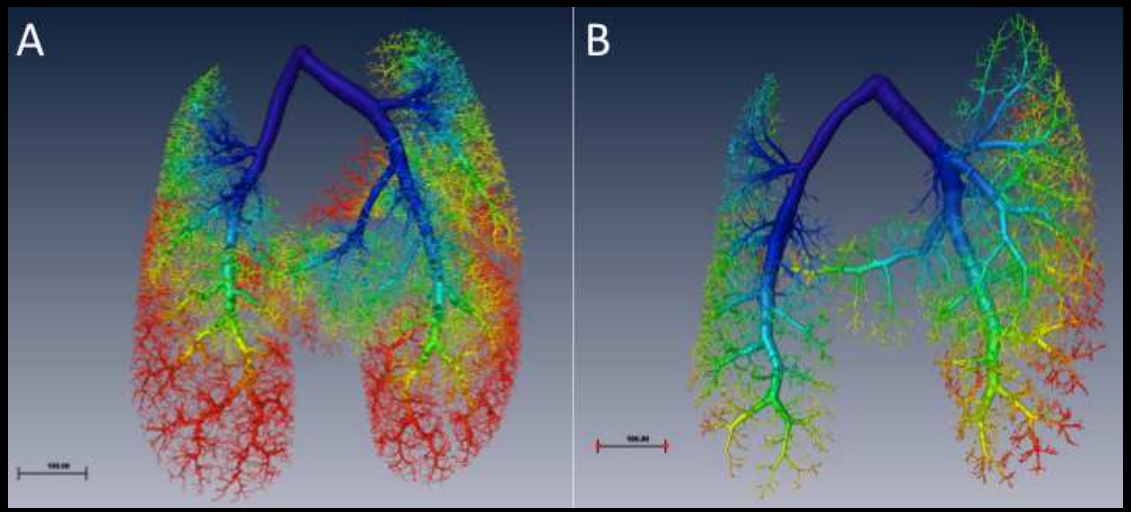
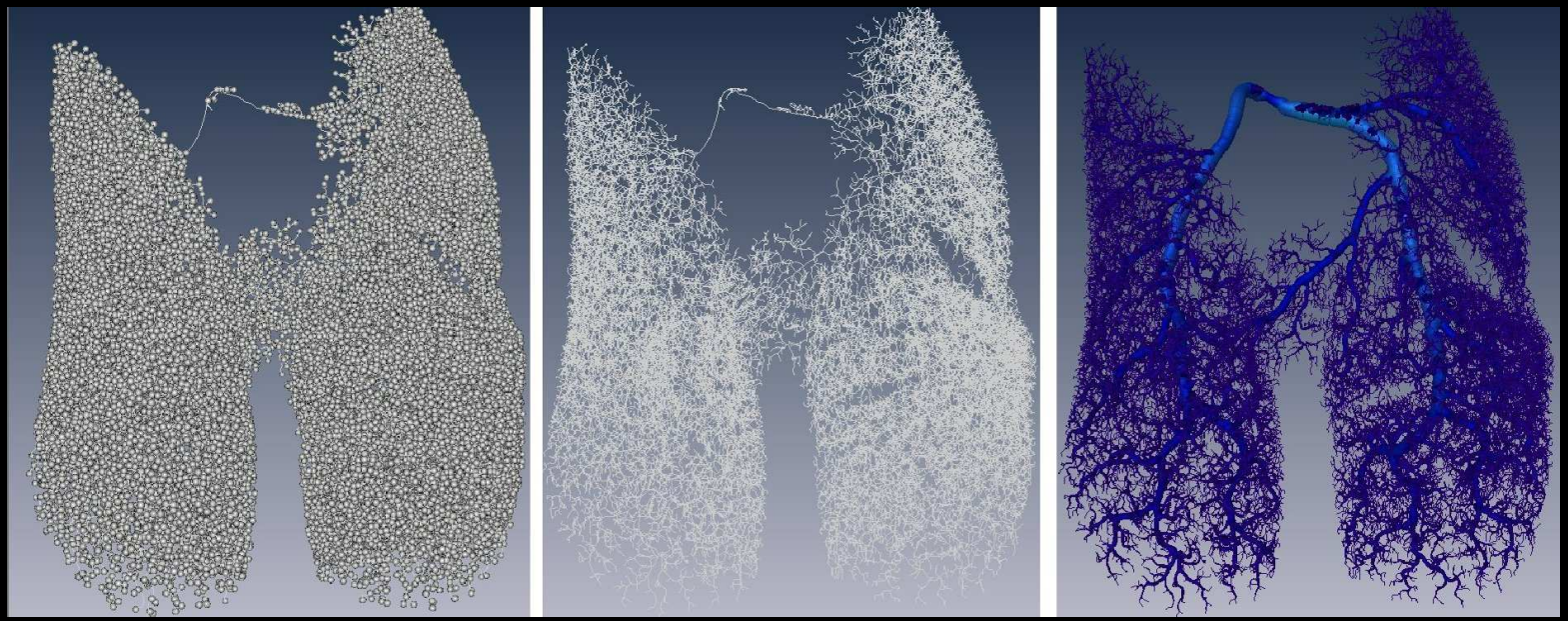
Lung airways (COPD study)



[Belchi, Pirashvili, Conway, Bennett, Djukanovic, Brodzki 2018]

Lung vessels (CDH study)





courtesy Sean McLean

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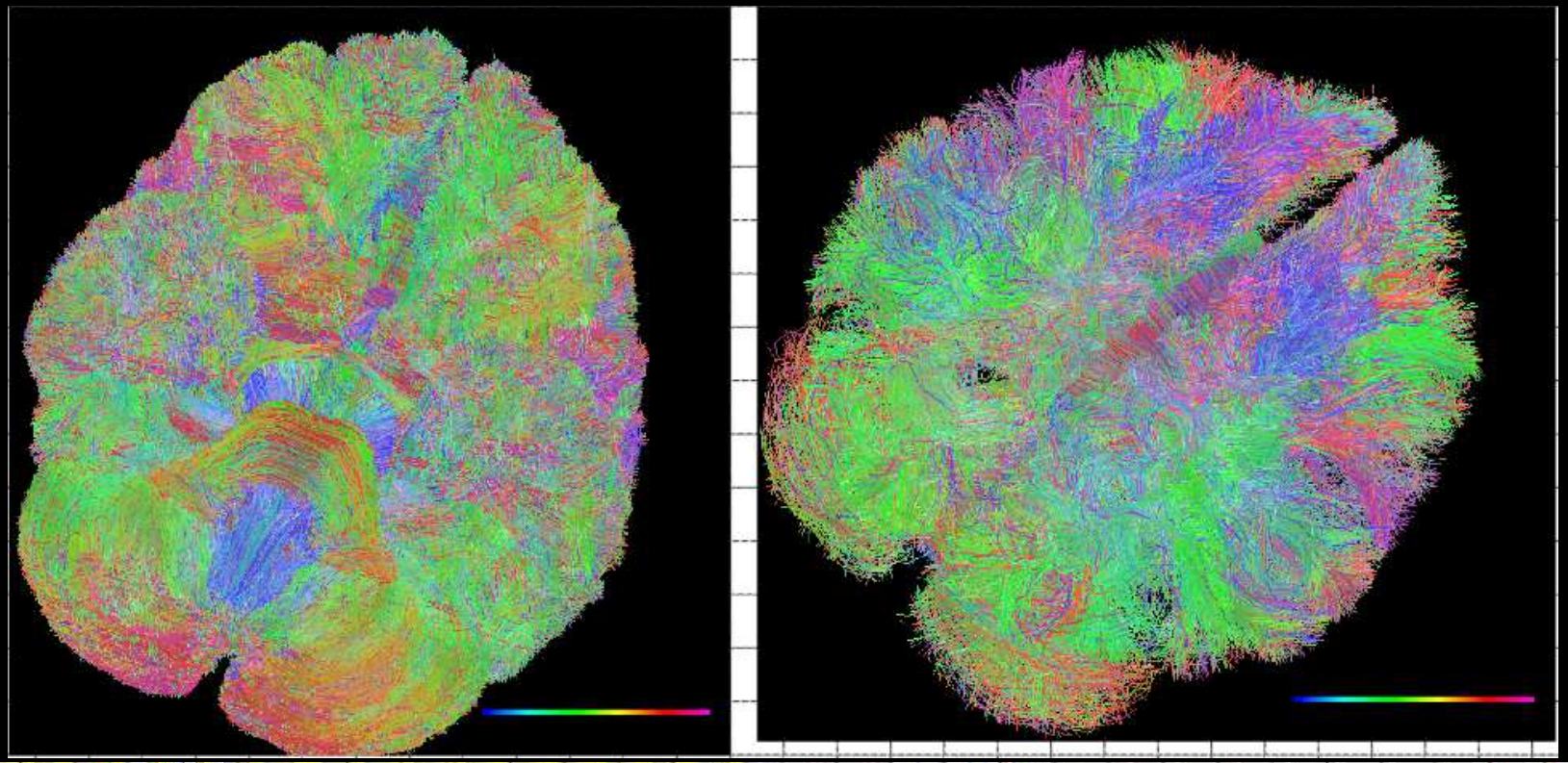
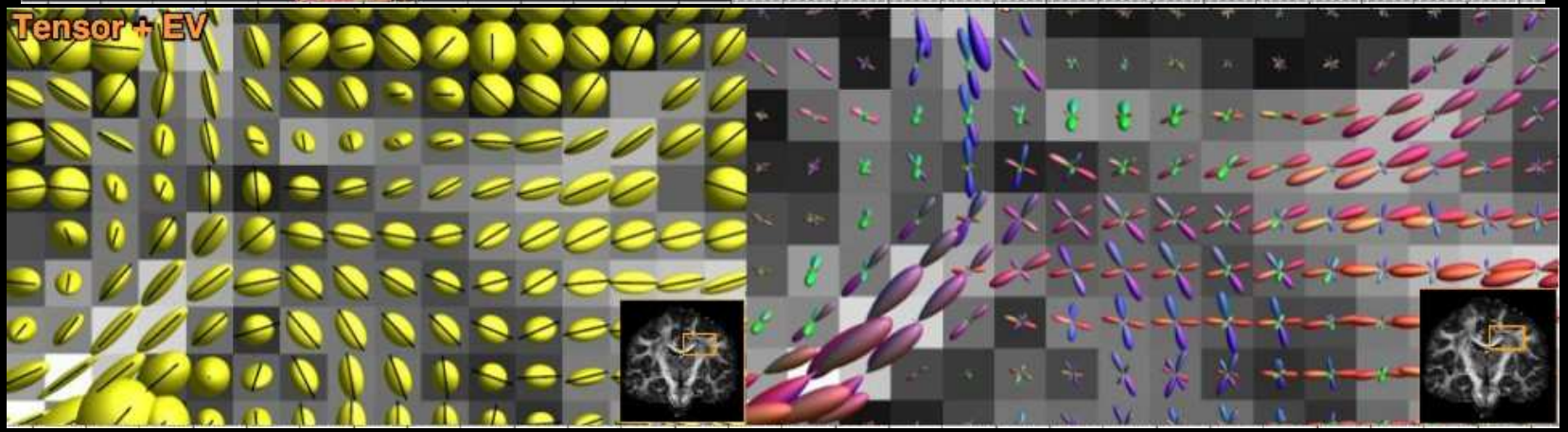
Streamlines from Diffusion Tensor Imaging





courtesy Zhengwu Zhang

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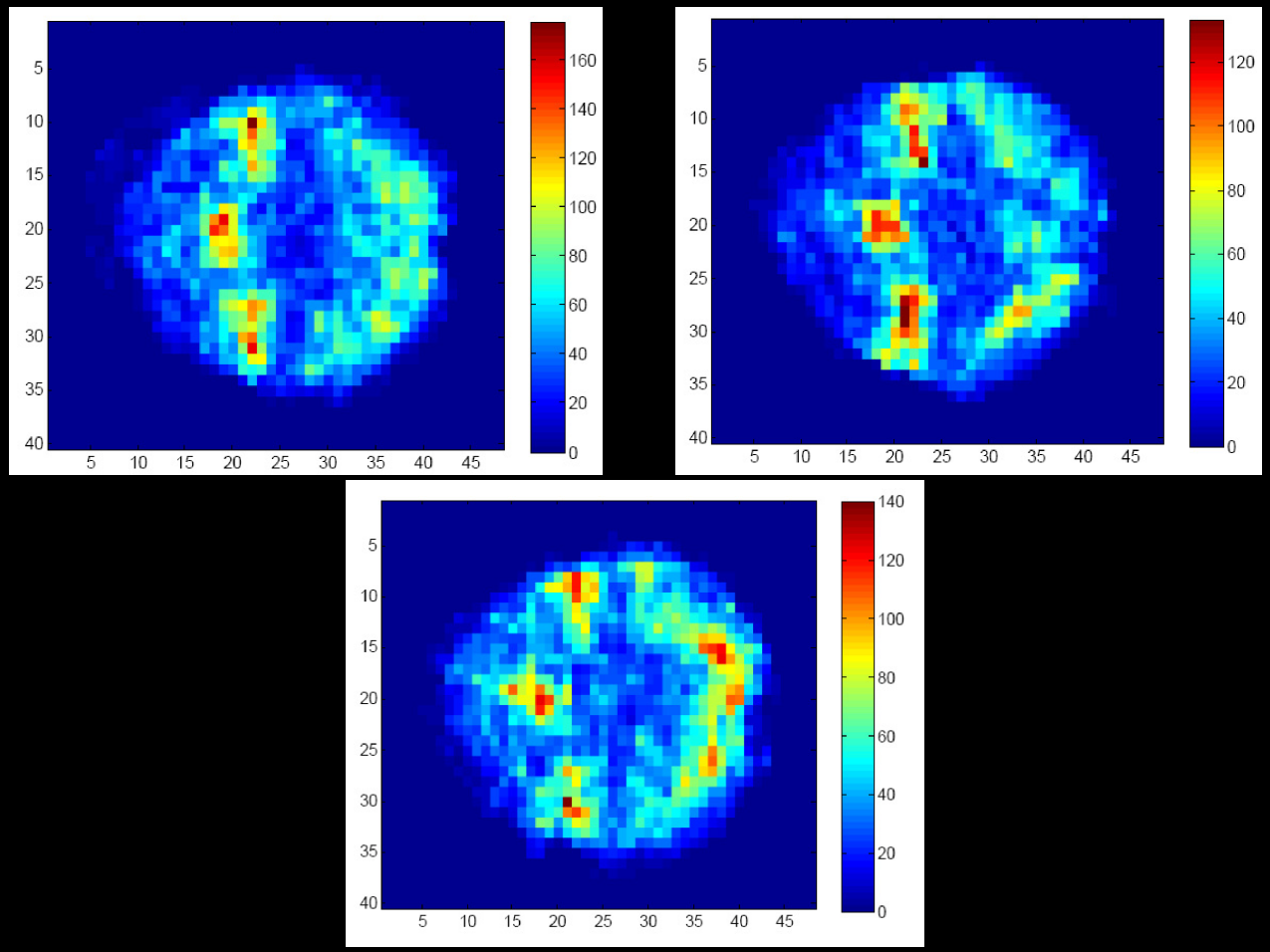

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Jamaica
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genus *Amphiacusta*

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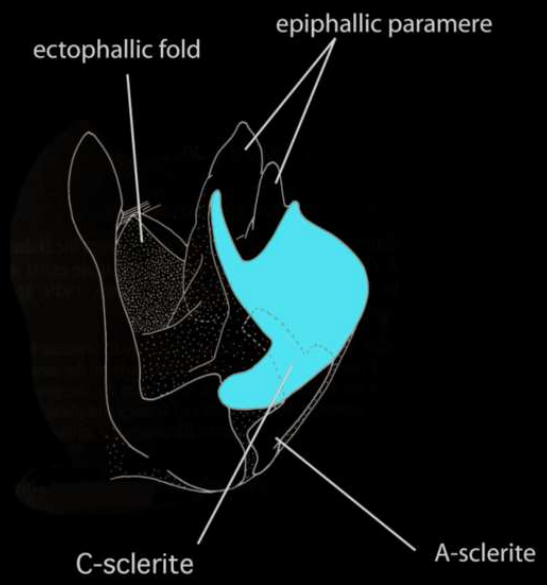
A. opsia
A. eritheles
A. annulipes
A. apoplanos
A. domingensis
A. exacerbans
A. extenta
A. mythica
A. pomierense
A. hespera
A. dapanera
A. obstipa
A. ominosa
A. dimalea
A. expansa
A. sterna
A. hyperphobos
A. sanctaecrucis
A. nauta
A. viequesense
A. lares
A. pronauta
A. tijicohniae
A. species 1
A. henrymorgani
A. ruizi
A. sincerus
Yoyuteris phacode

0.1 substitutions/site



From Oneal, Otte & Knowles, 2010

Drawings by Dan Otte

What kinds of data?

Shapes

- 1D: curves (in $\mathbb{R}^2$ or $\mathbb{R}^3$, say)
- 2D: photographs
- 3D: MRI, DTI, SPECT, PET, CAT, integrated photo
  - cricket sclerites
  - brain arteries
  - lung airways
  - fiber tracts
- (2+1)D: video (.mp4, .mov, ...)
- 4D: fMRI, or any time series of spatial 3D
- arbitrary D: abstract geometric structures from data
  - any bunch of isolated points in $\mathbb{R}^n$ (!), especially for $n \gg 0$
  - any reasonable probability distribution

Networks

- neurological
- metabolic
- regulatory (genetic)
- phylogenetic
- physical: road maps, plant roots, neuronal (dendritic), ...

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Persistent homology

Input. Topological space X filtered by set Q of subspaces: $X_q \subseteq X$ for $q \in Q$

$\Rightarrow Q$ is a partially ordered set: $X_q \subseteq X_{q'} \Leftrightarrow q \preceq q'$

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Examples

- points in $\mathbb{R}^n$: $Q = \{0, \ldots, m\}$ or $\mathbb{R}$ 1-parameter ("ordinary") persistence
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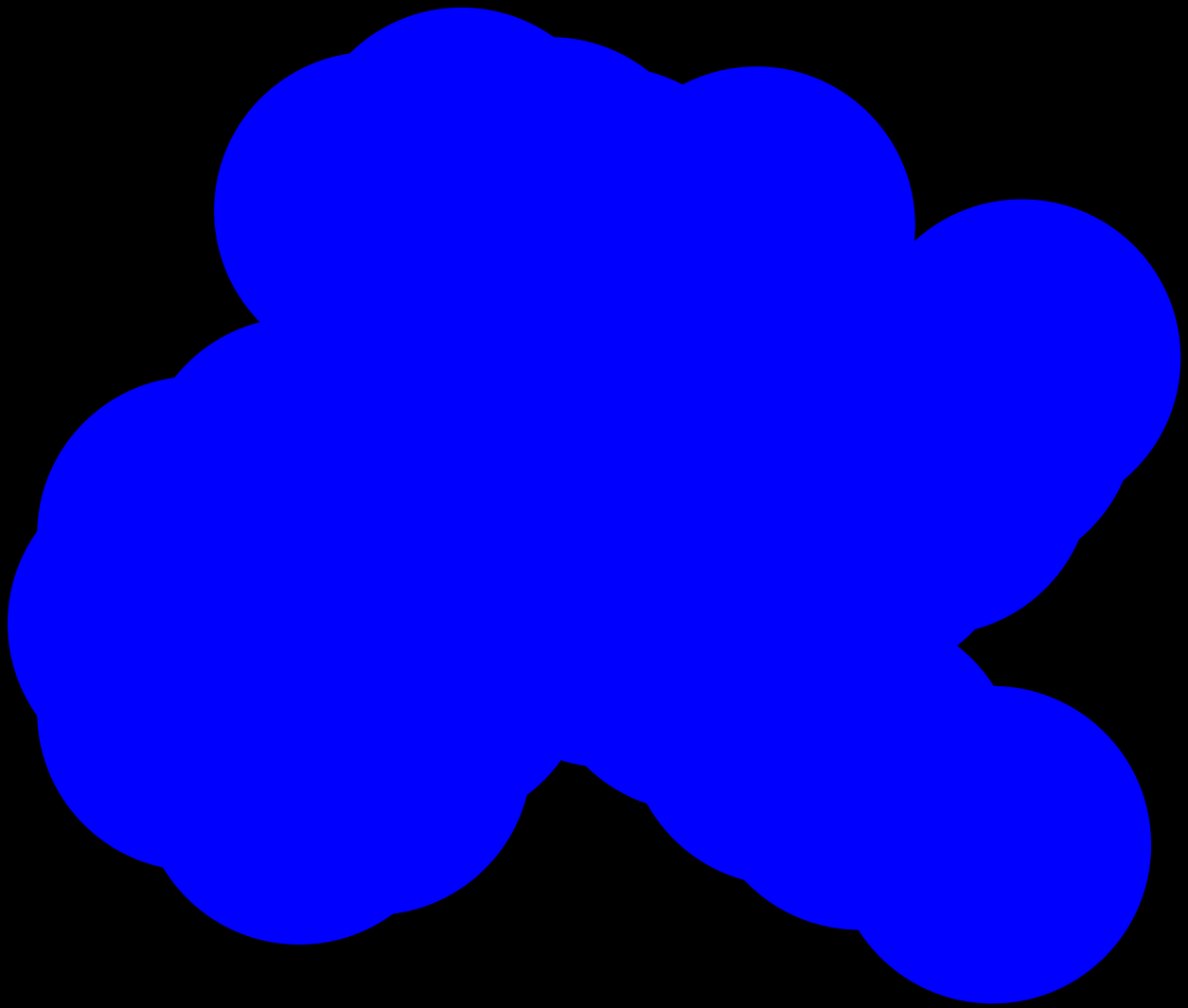
Example: expanding balls



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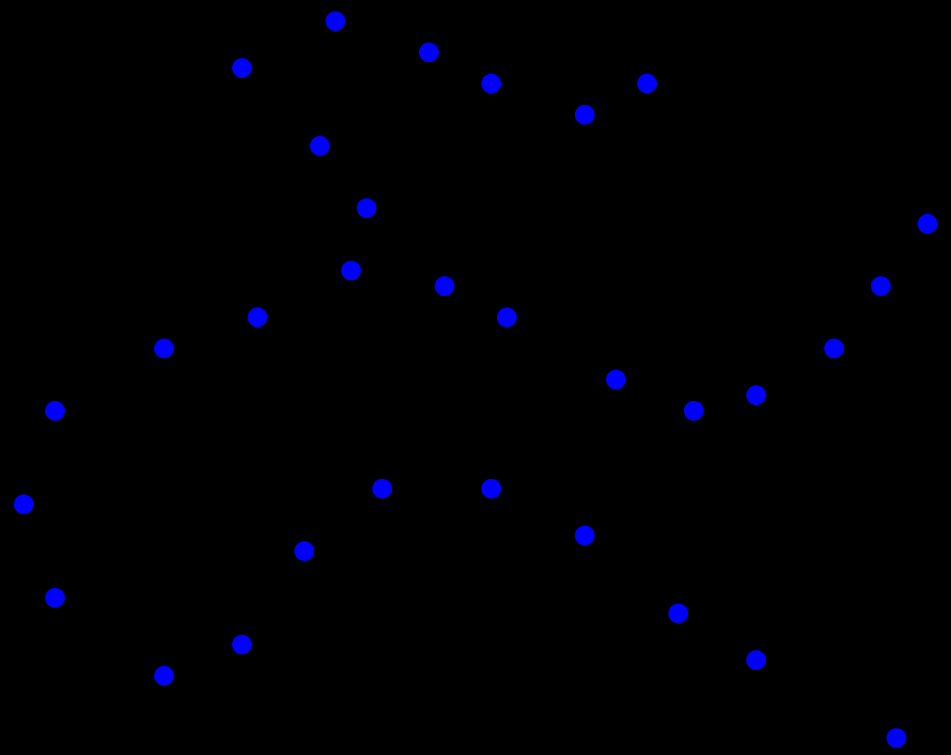

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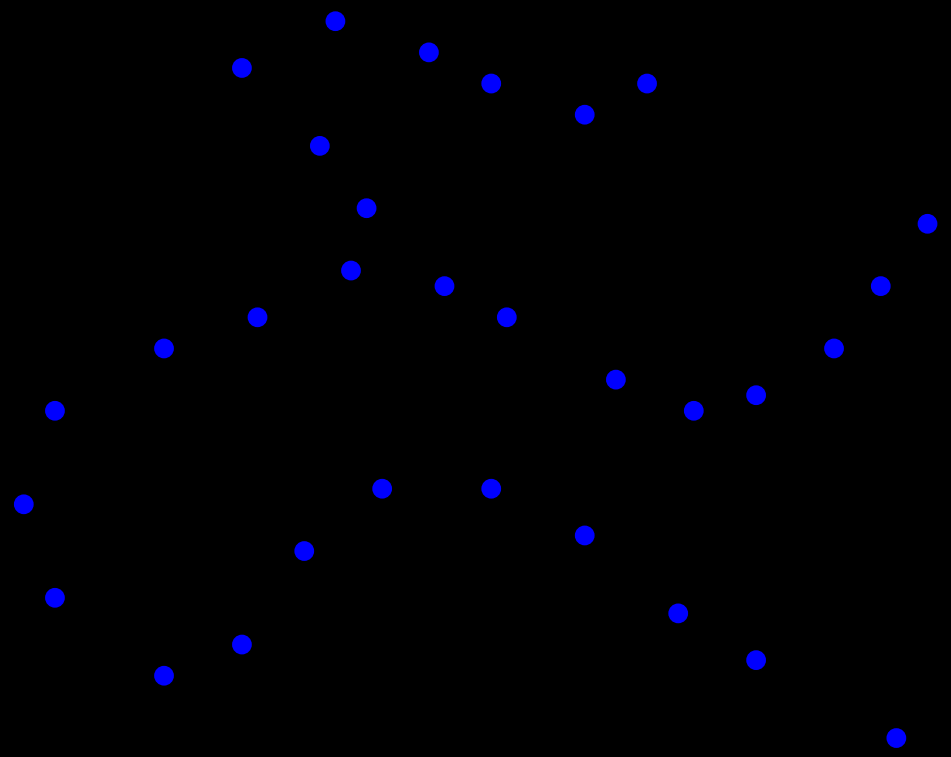

$\dim(H_0) = 31$

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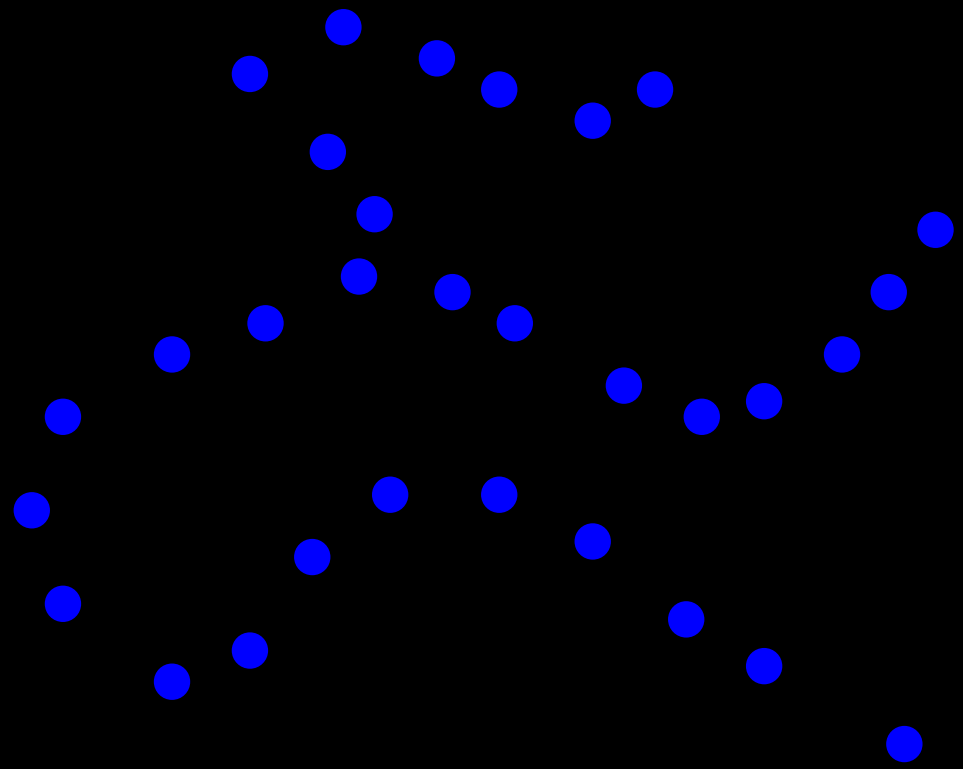

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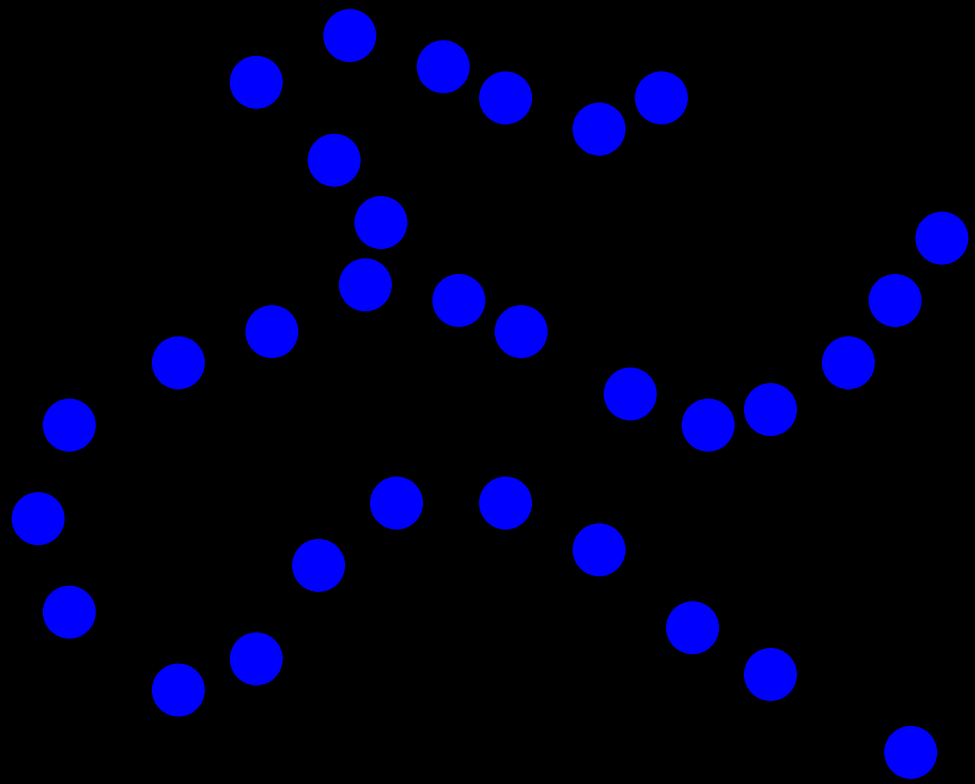

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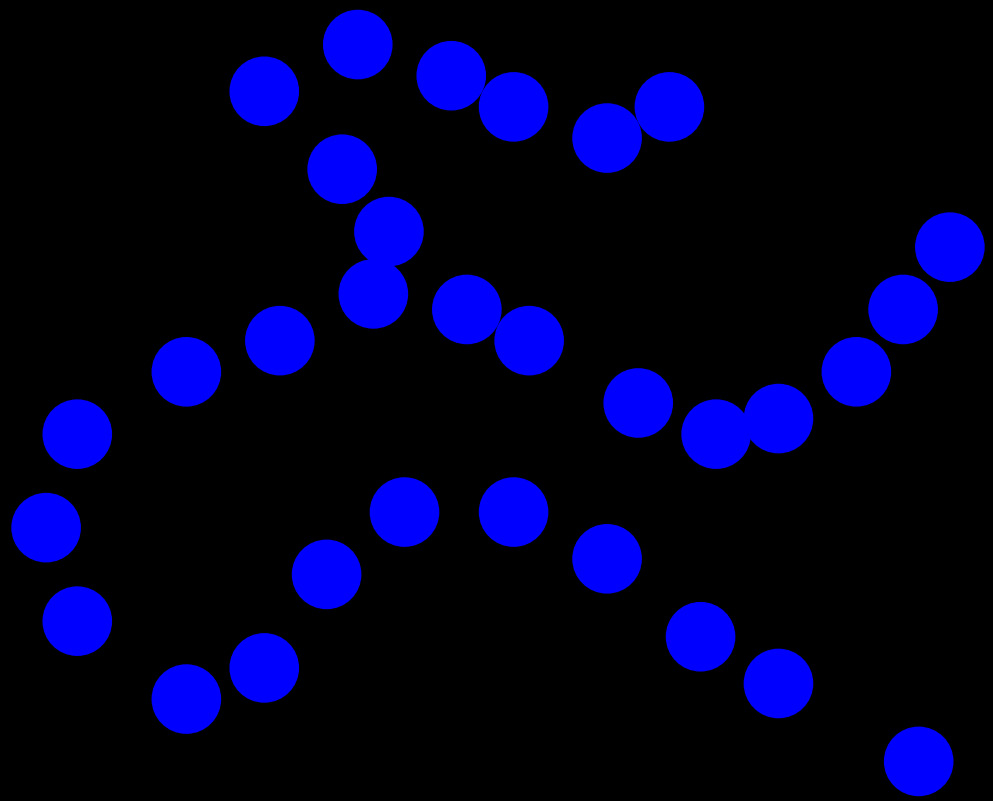
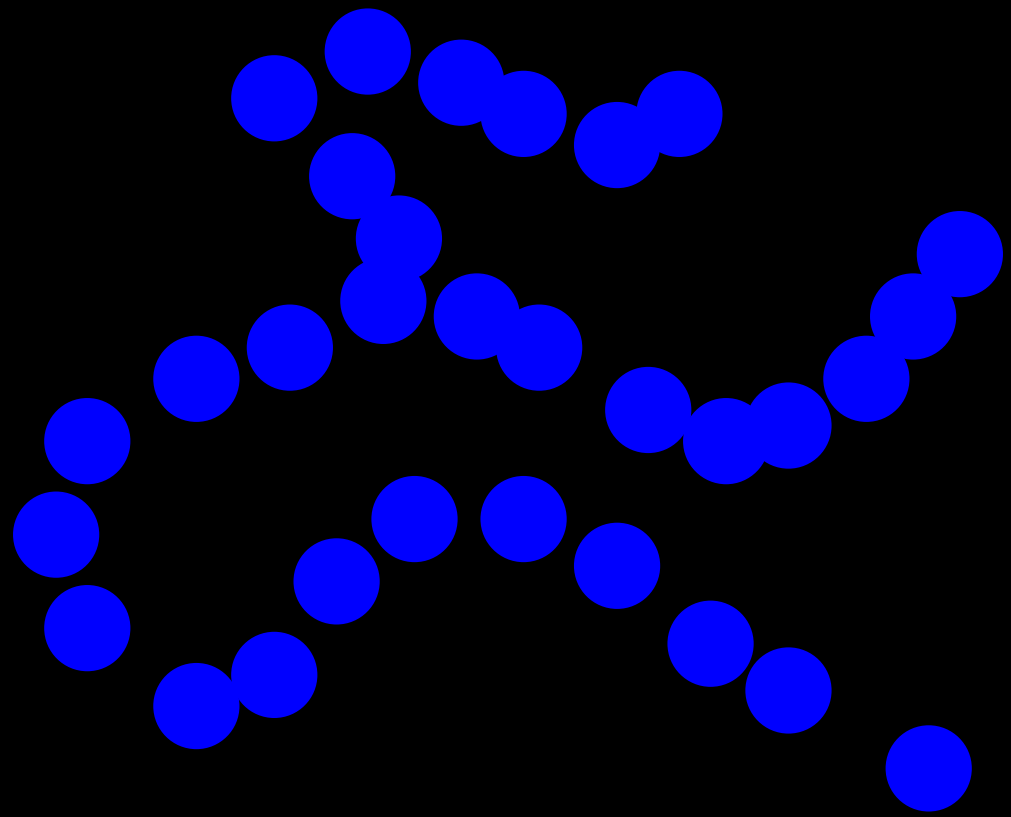


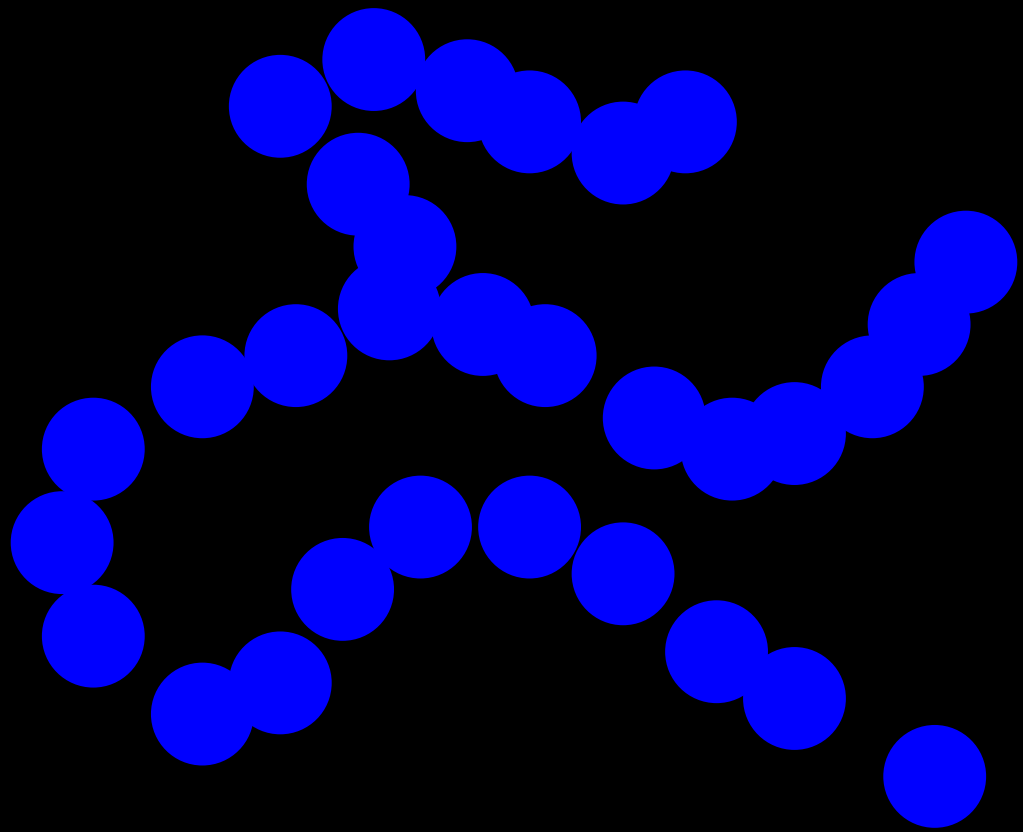
$\dim(H_0) = 26$

Example: expanding balls



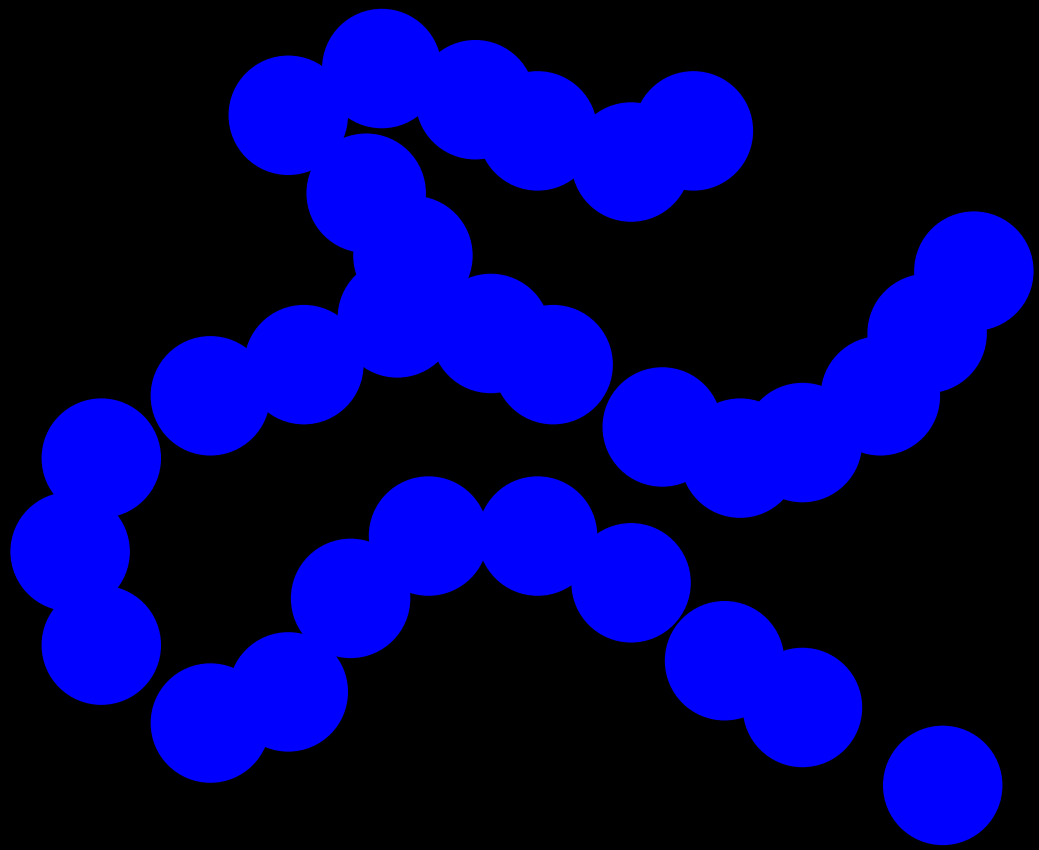
$\dim(H_0) = 21$

Example: expanding balls



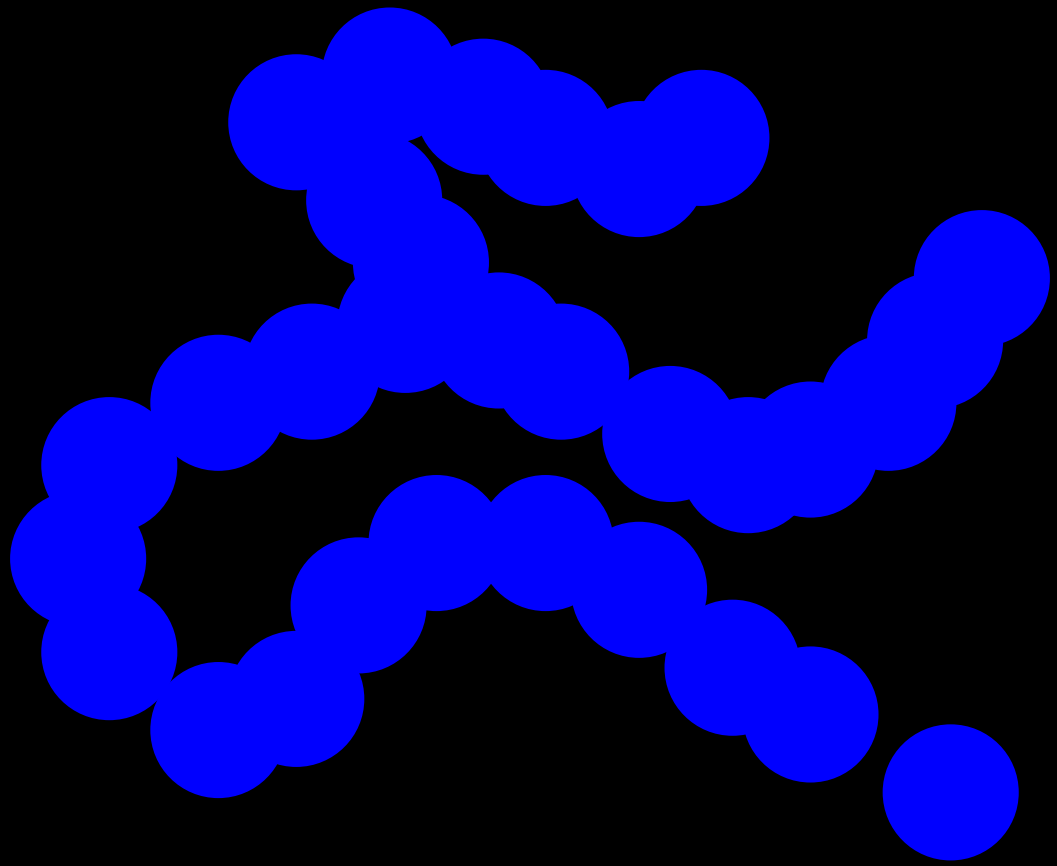
$\dim(H_0) = 12$

Example: expanding balls



$\dim(H_0) = 6$

Example: expanding balls



$\dim(H_0) = 2$

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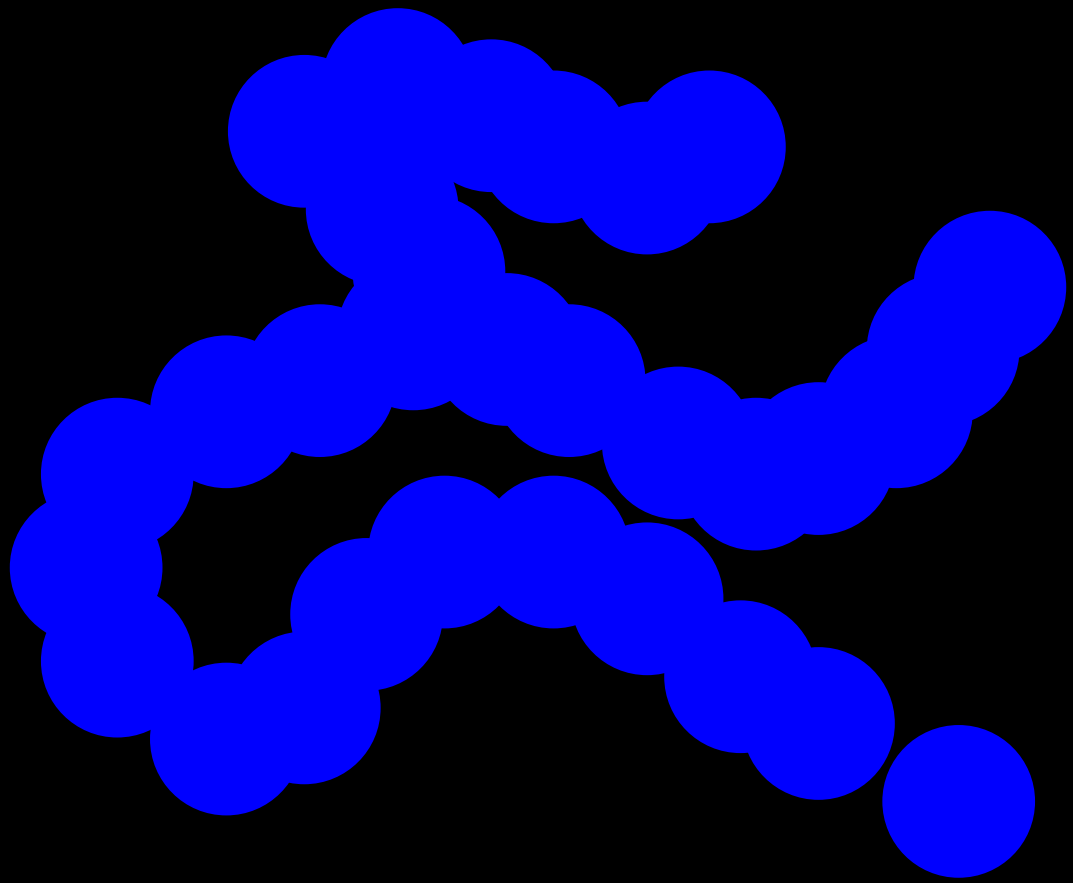

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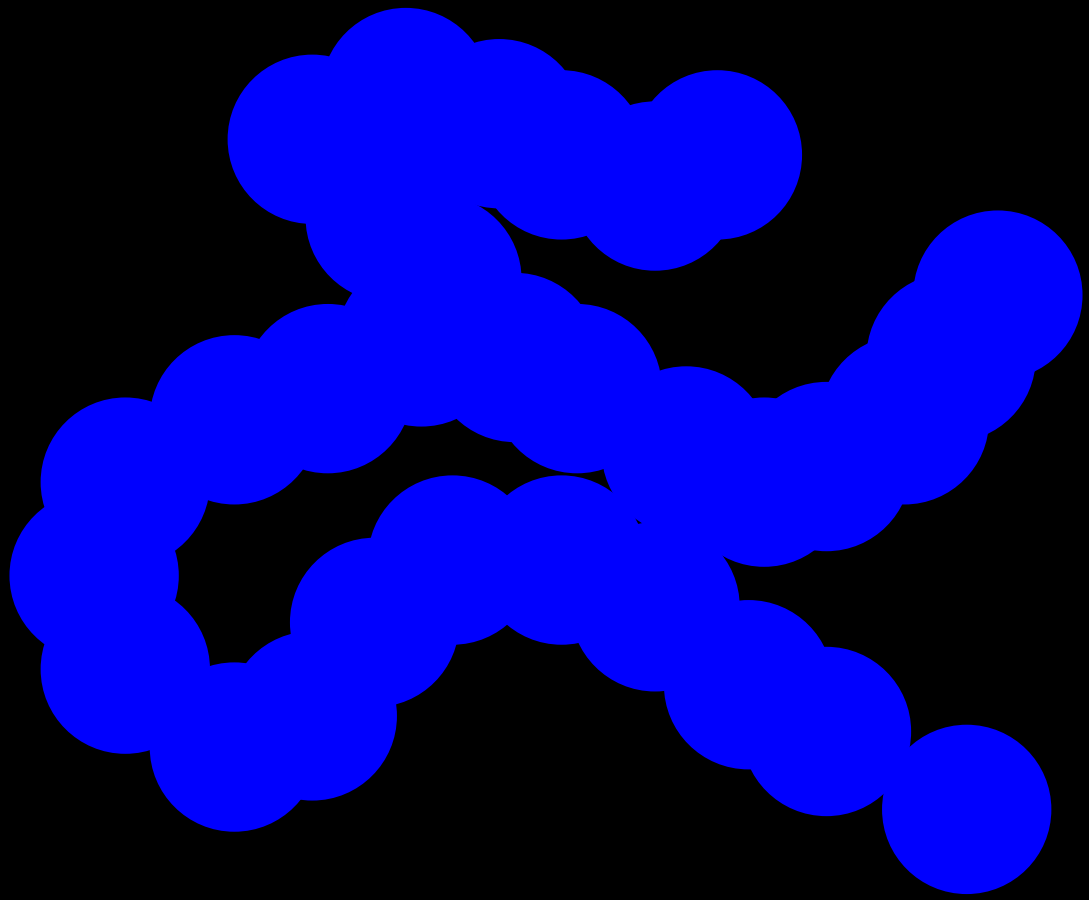
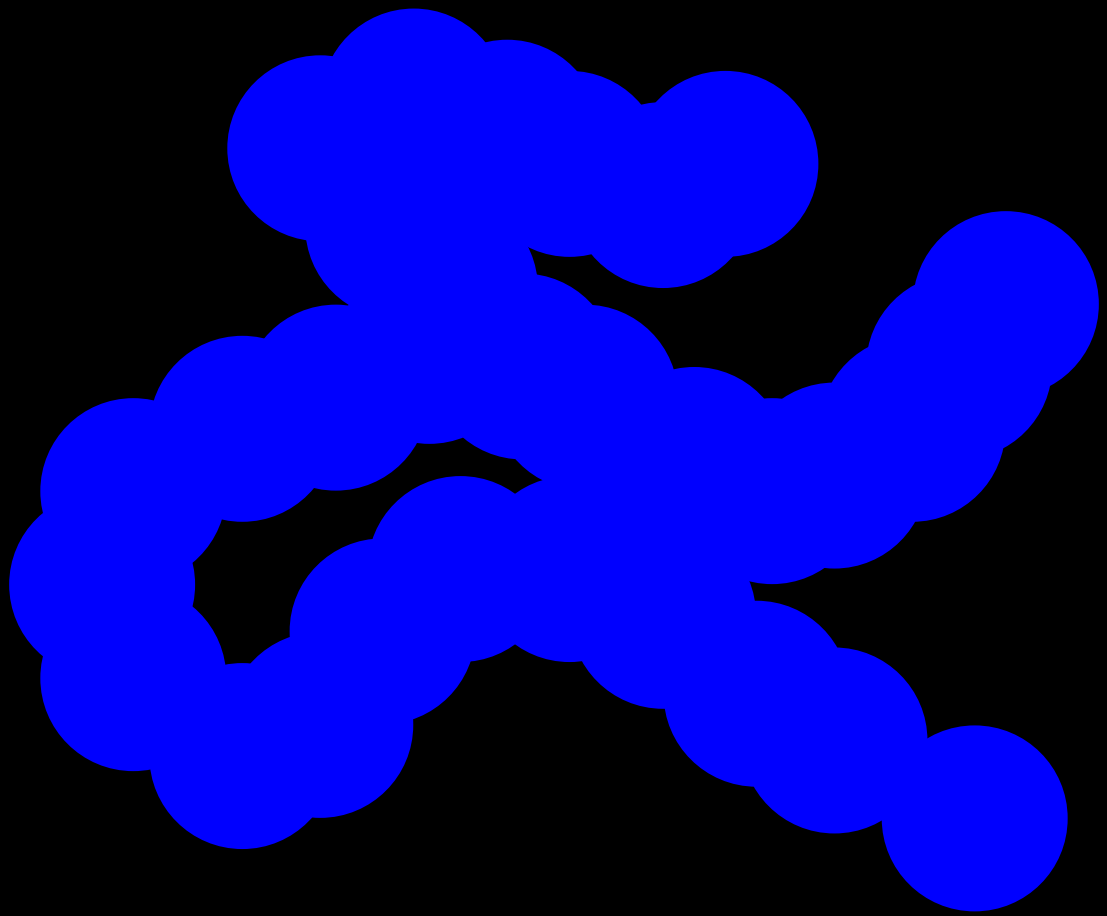


$\dim(H_0) = 1 \qquad \dim(H_1) = 2$

Example: expanding balls



$\dim(H_0) = 1 \qquad \dim(H_1) = 1$

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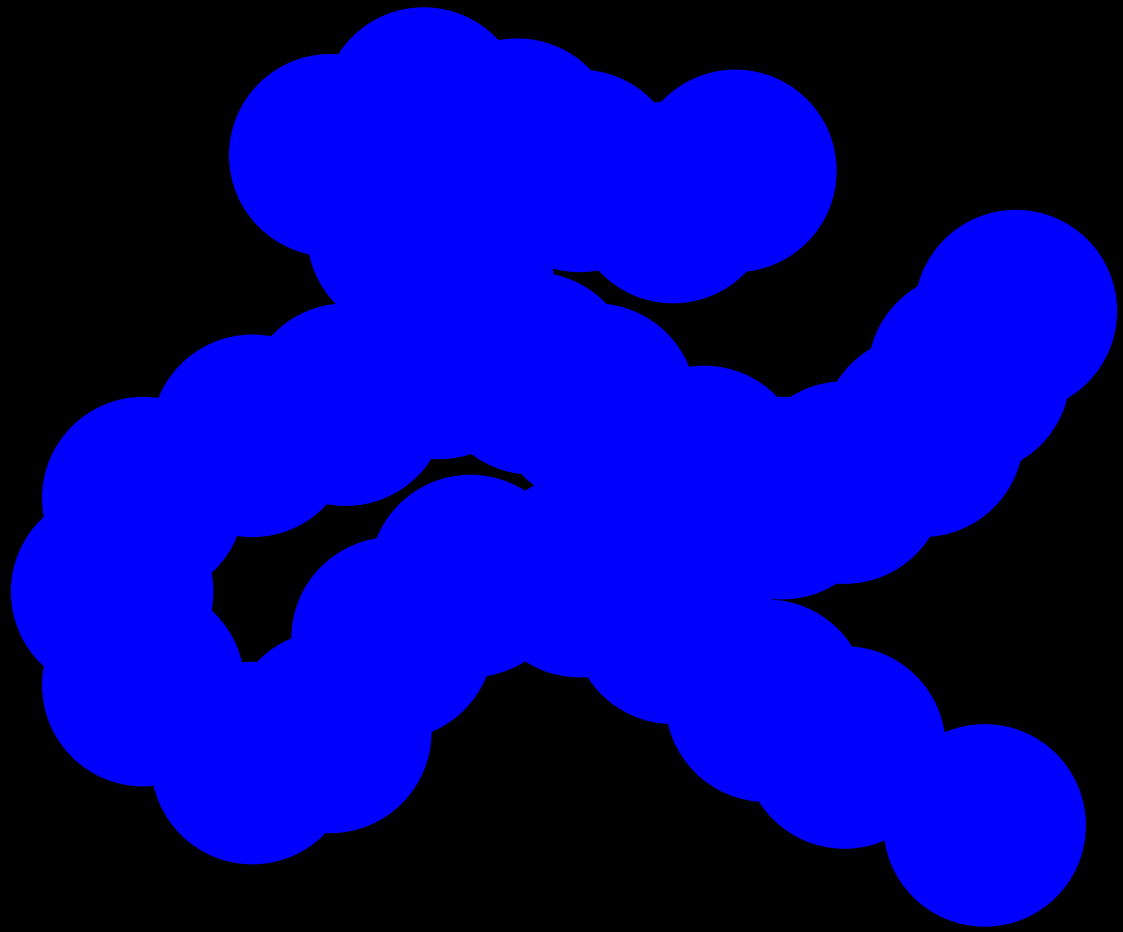

$\dim(H_0) = 1 \qquad \dim(H_1) = 1$

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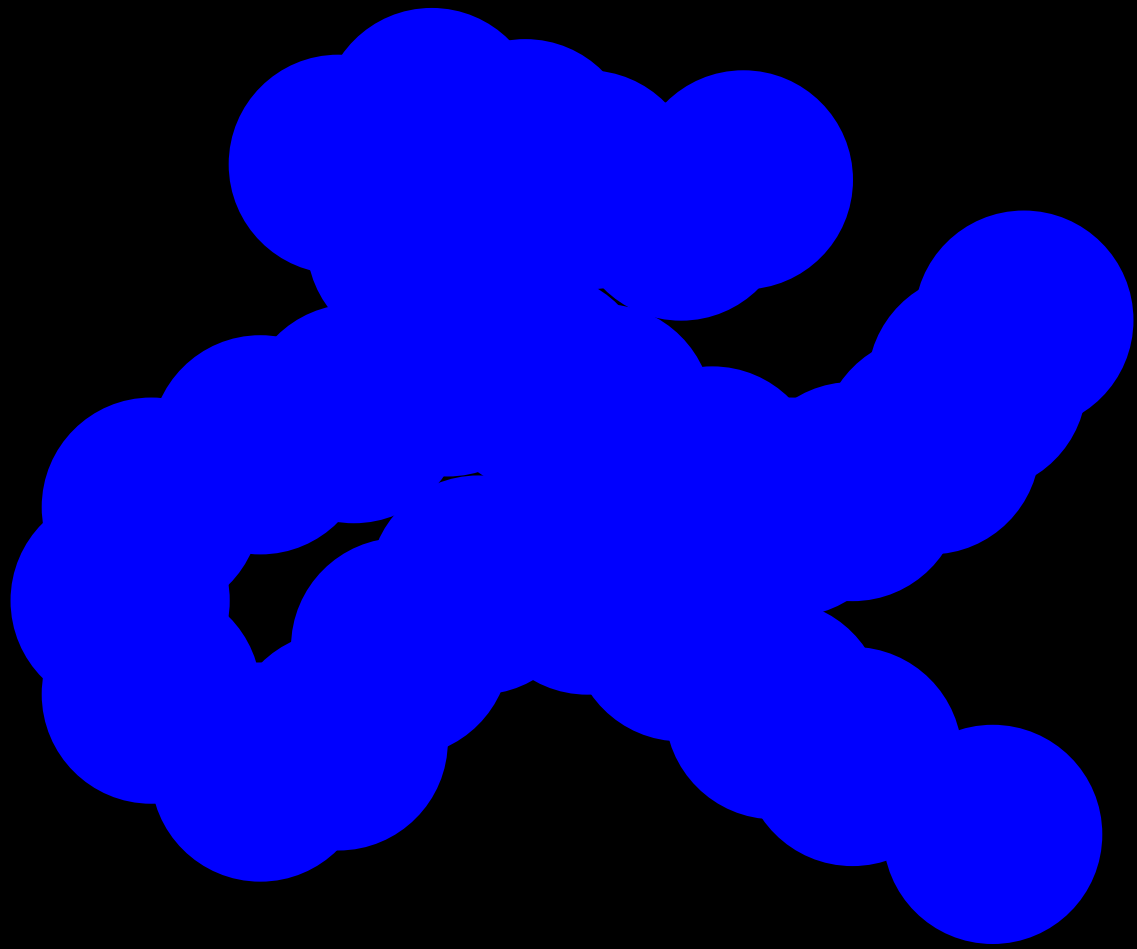

$\dim(H_0) = 1 \qquad \dim(H_1) = 3$

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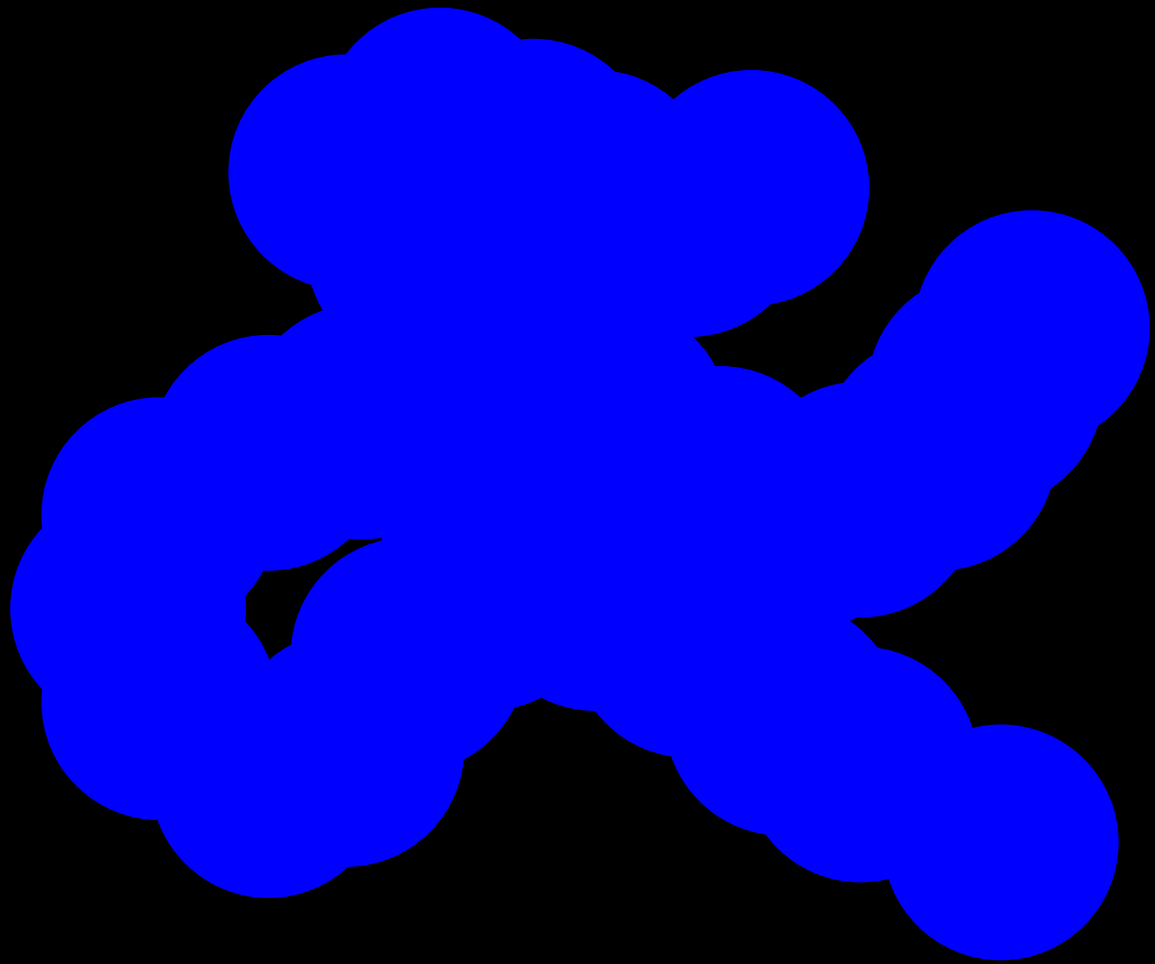

$\dim(H_0) = 1 \qquad \dim(H_1) = 1$

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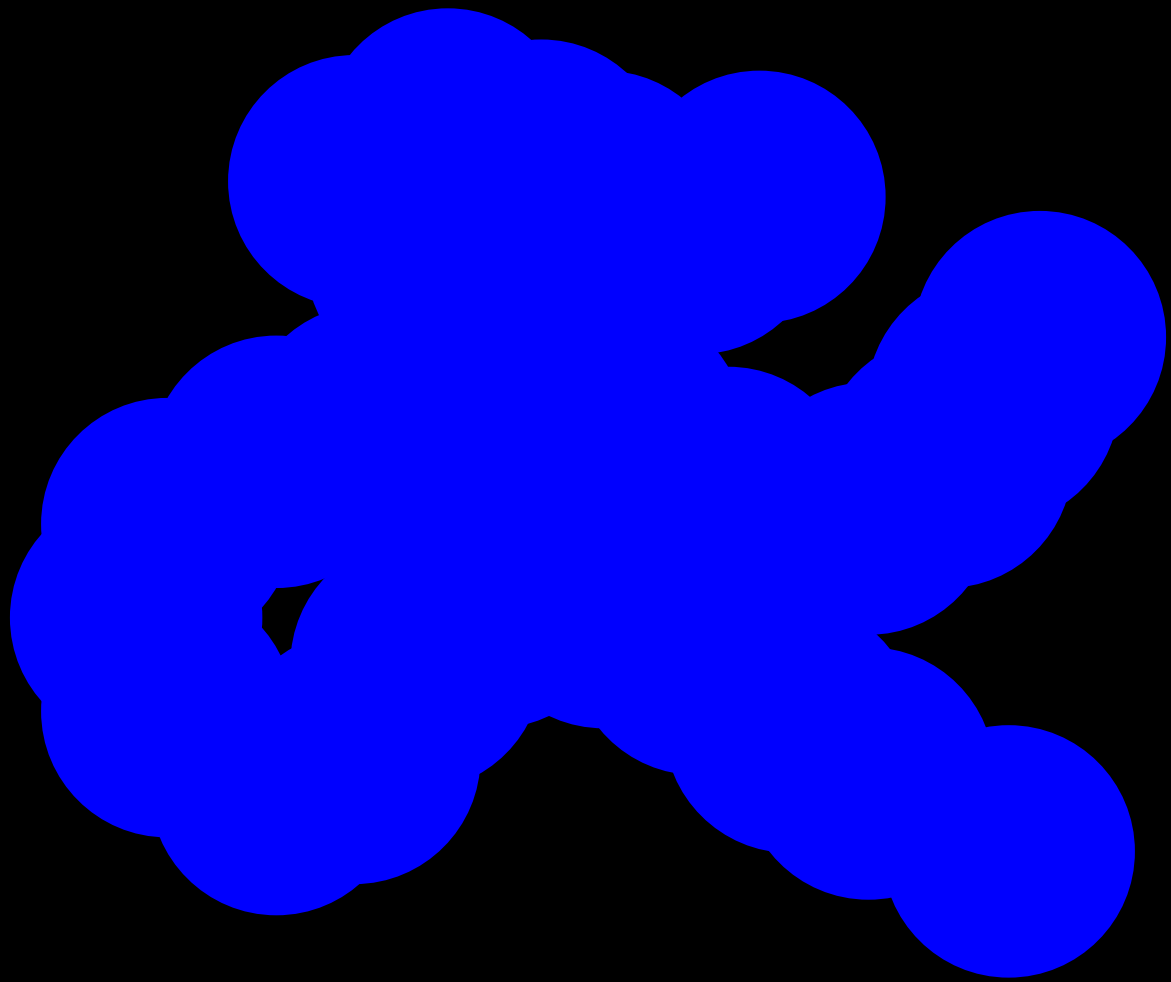

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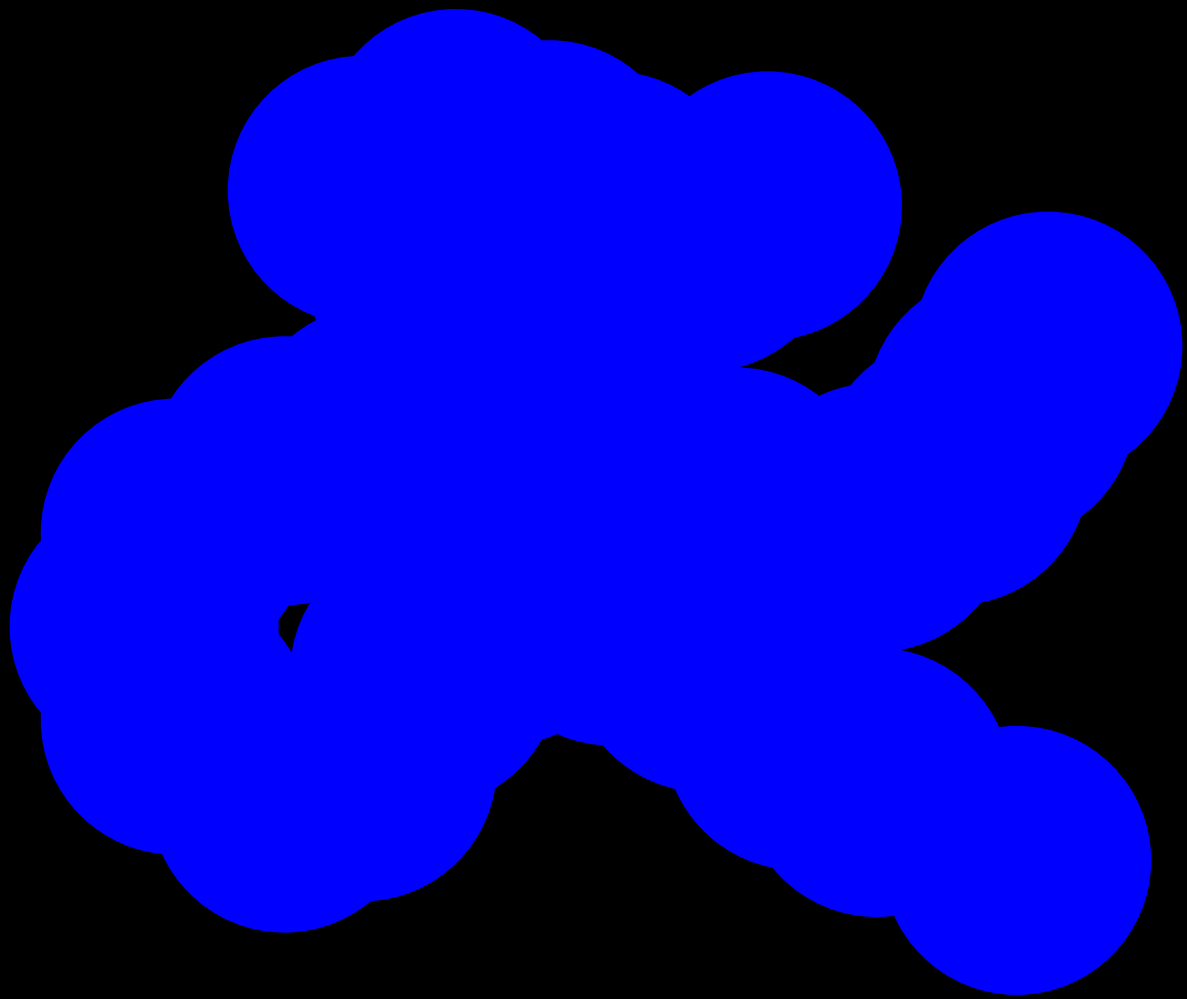

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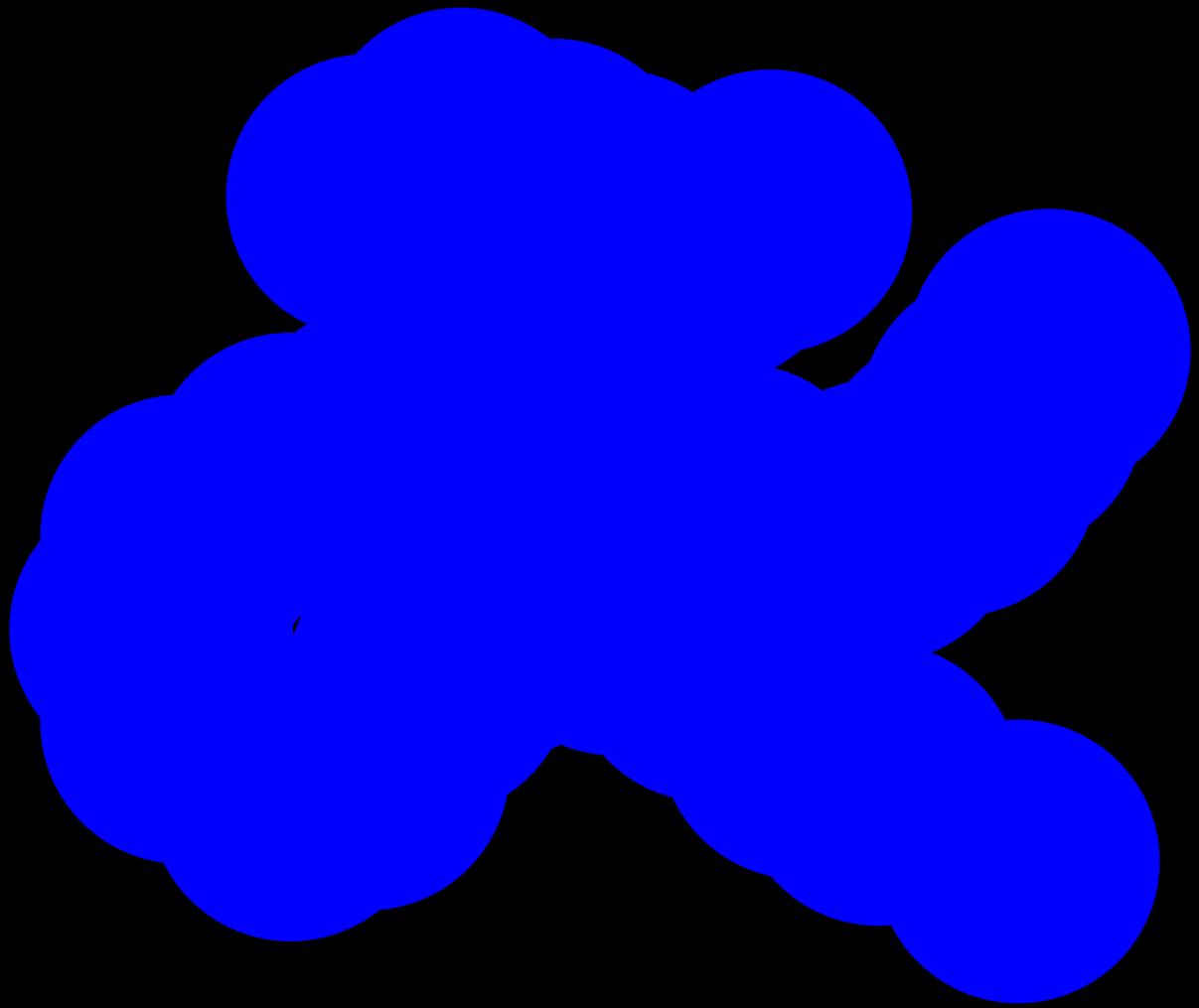

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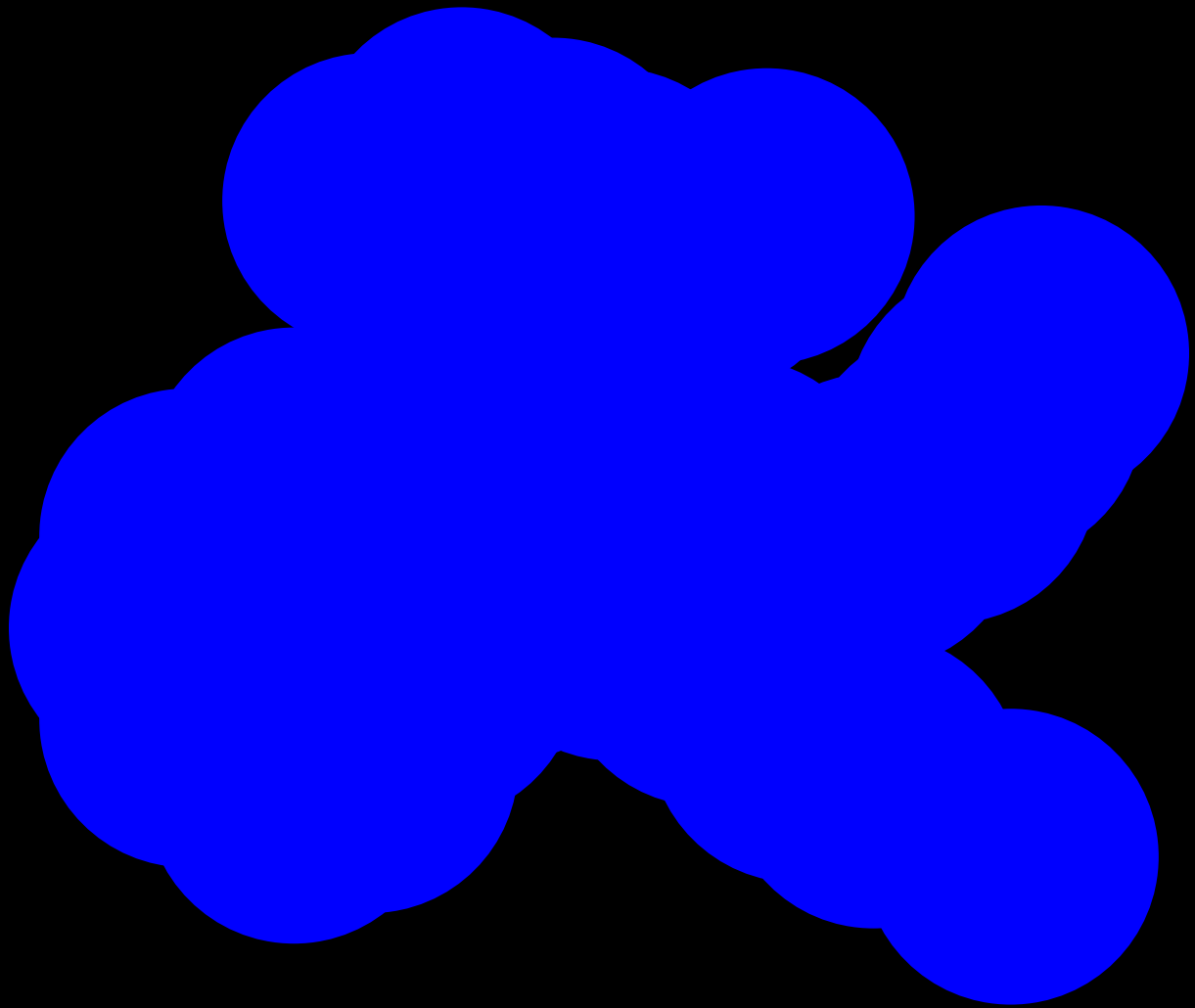

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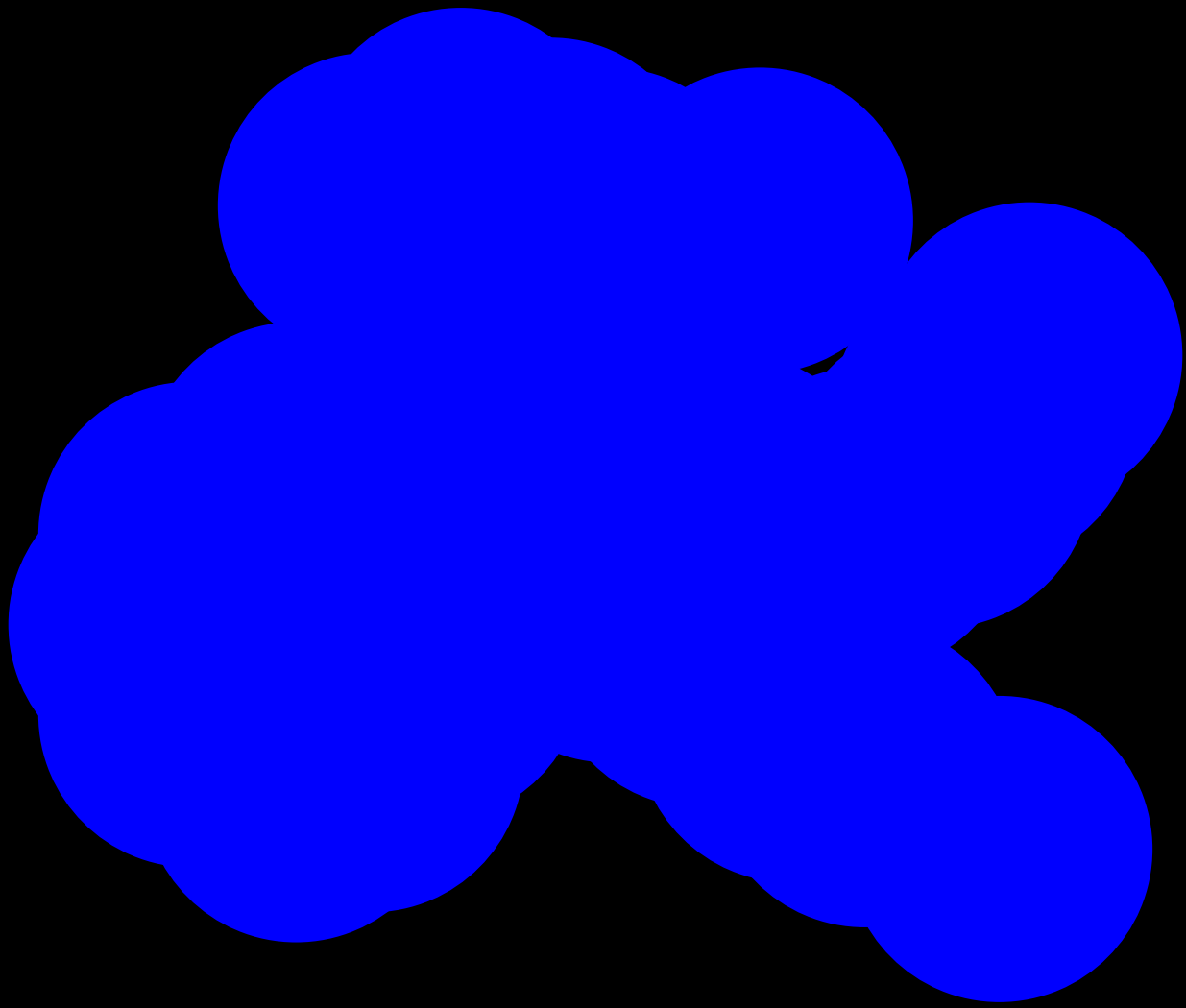

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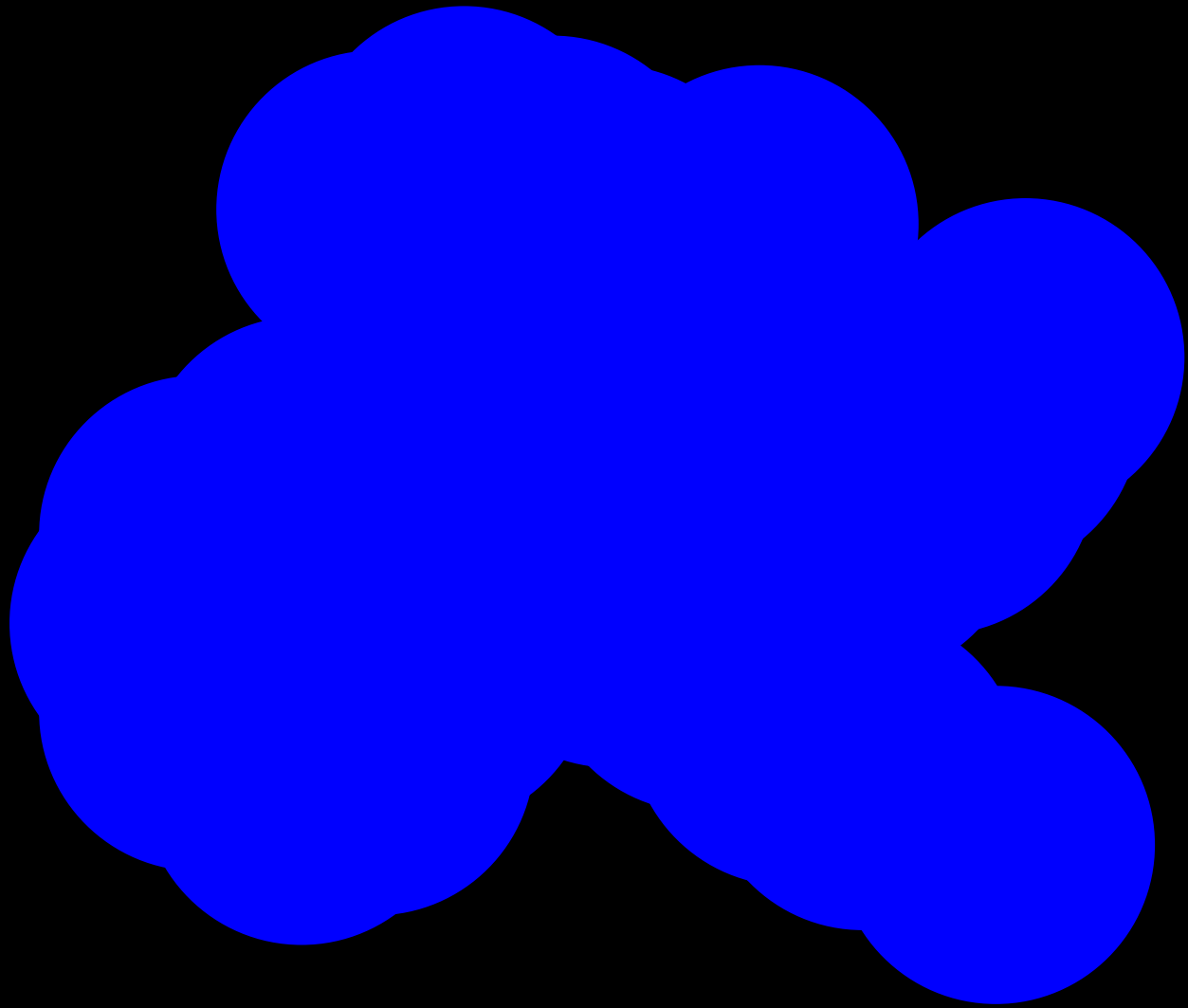

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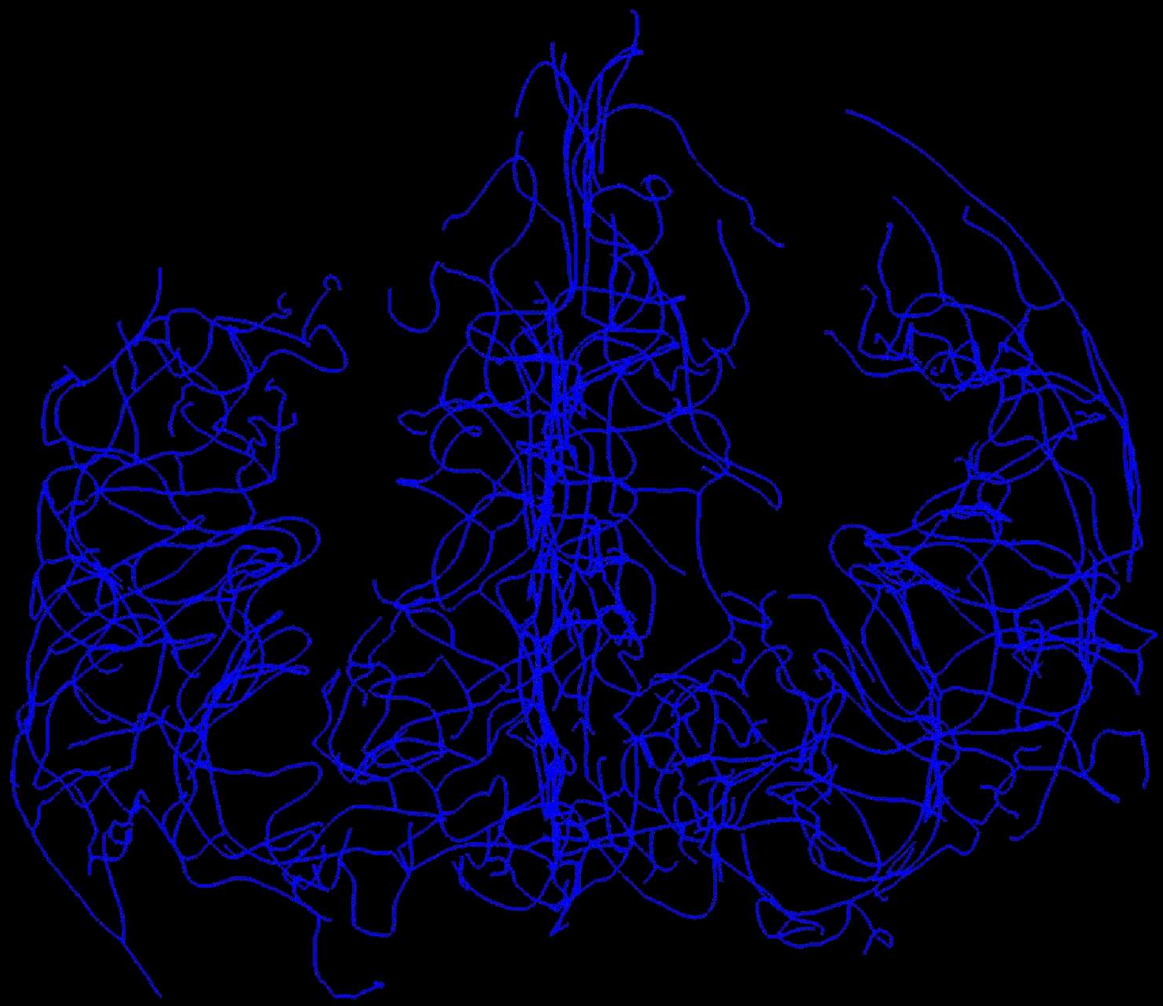

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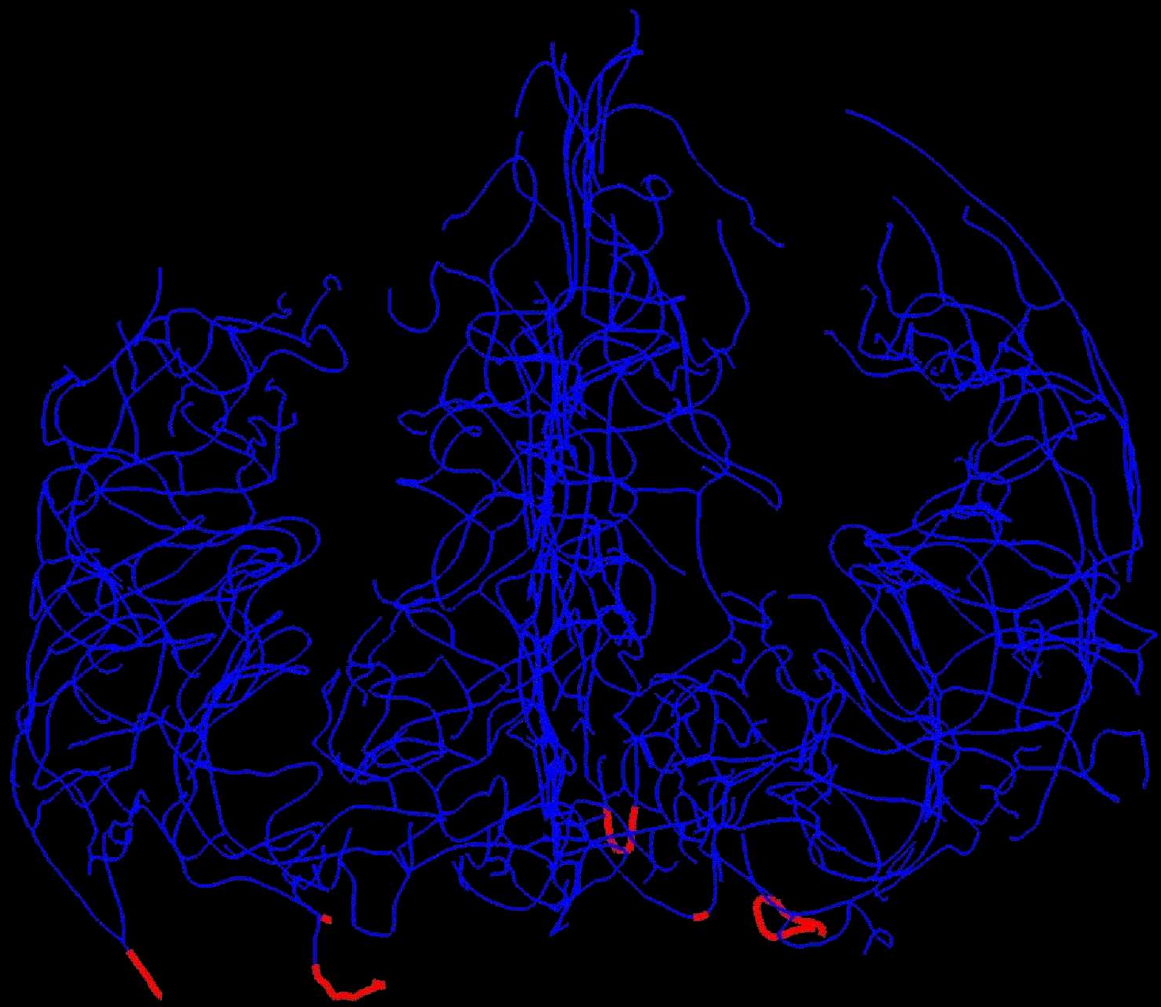

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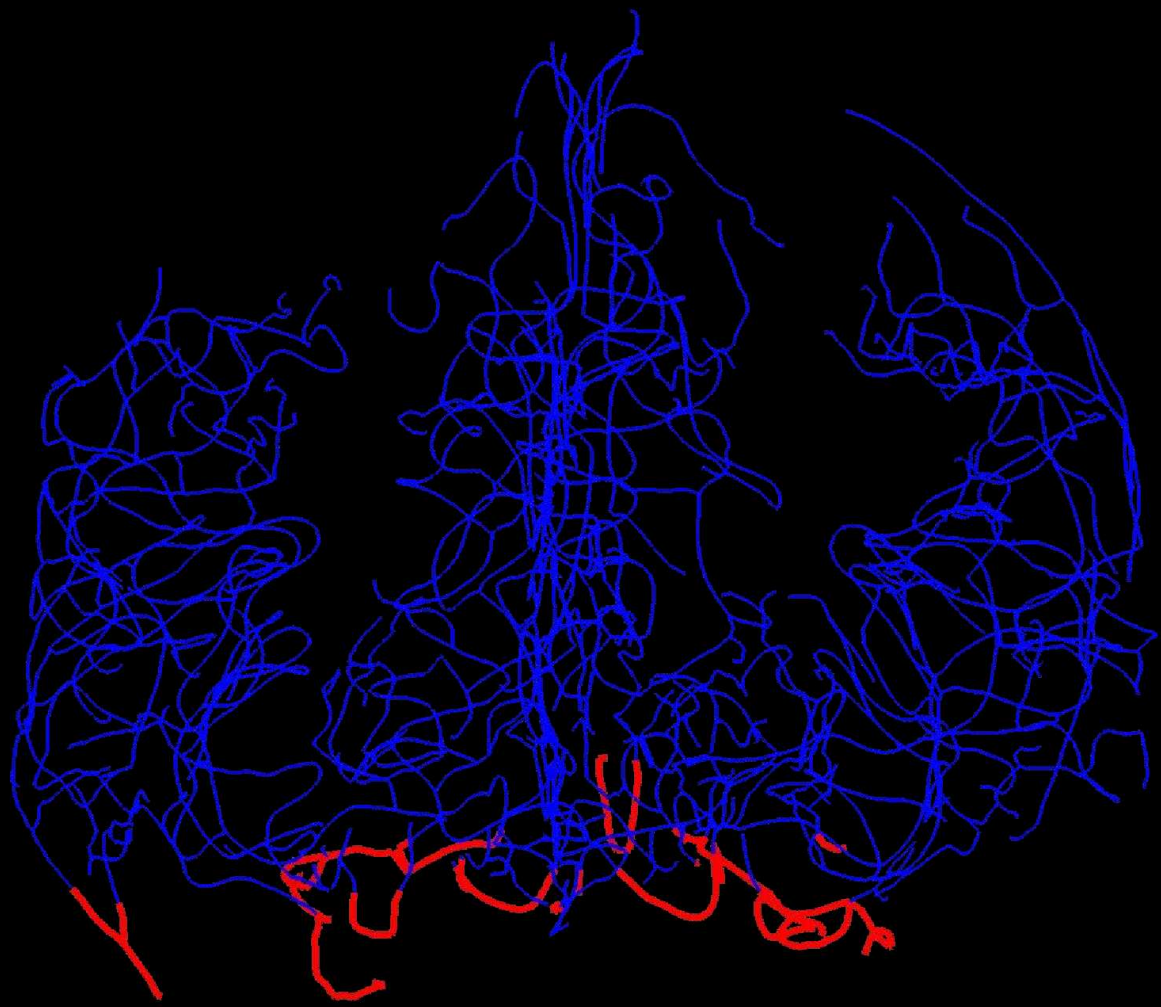

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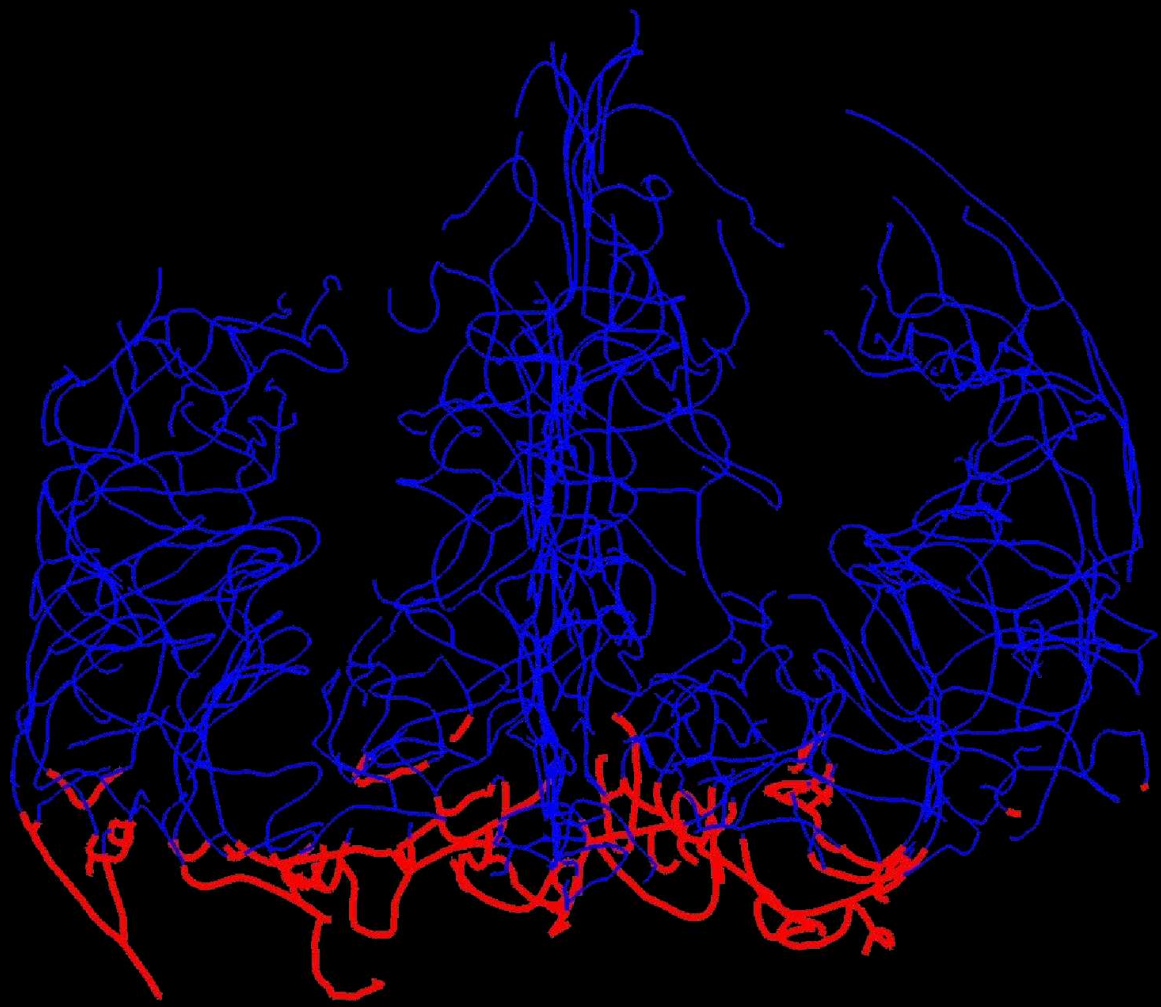

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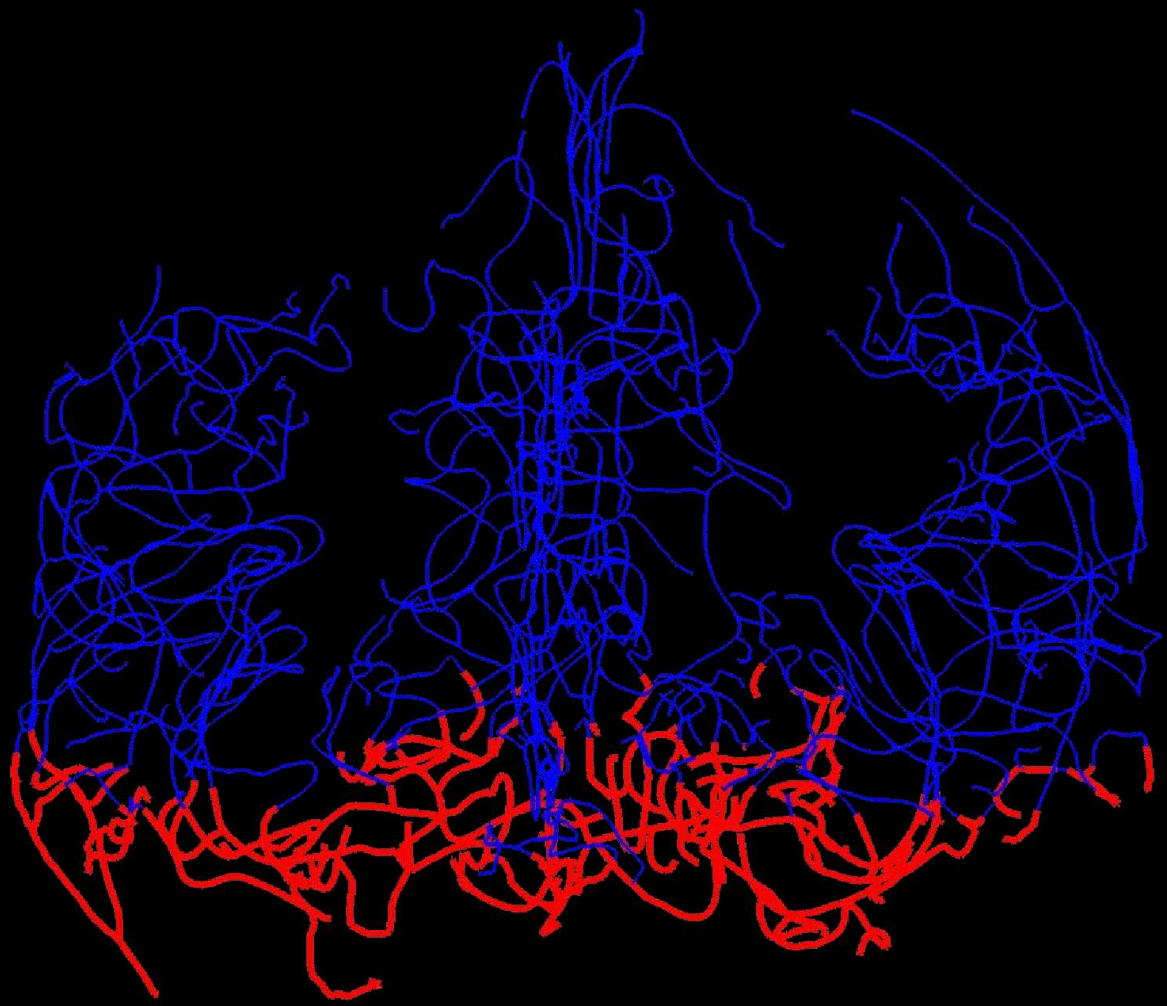

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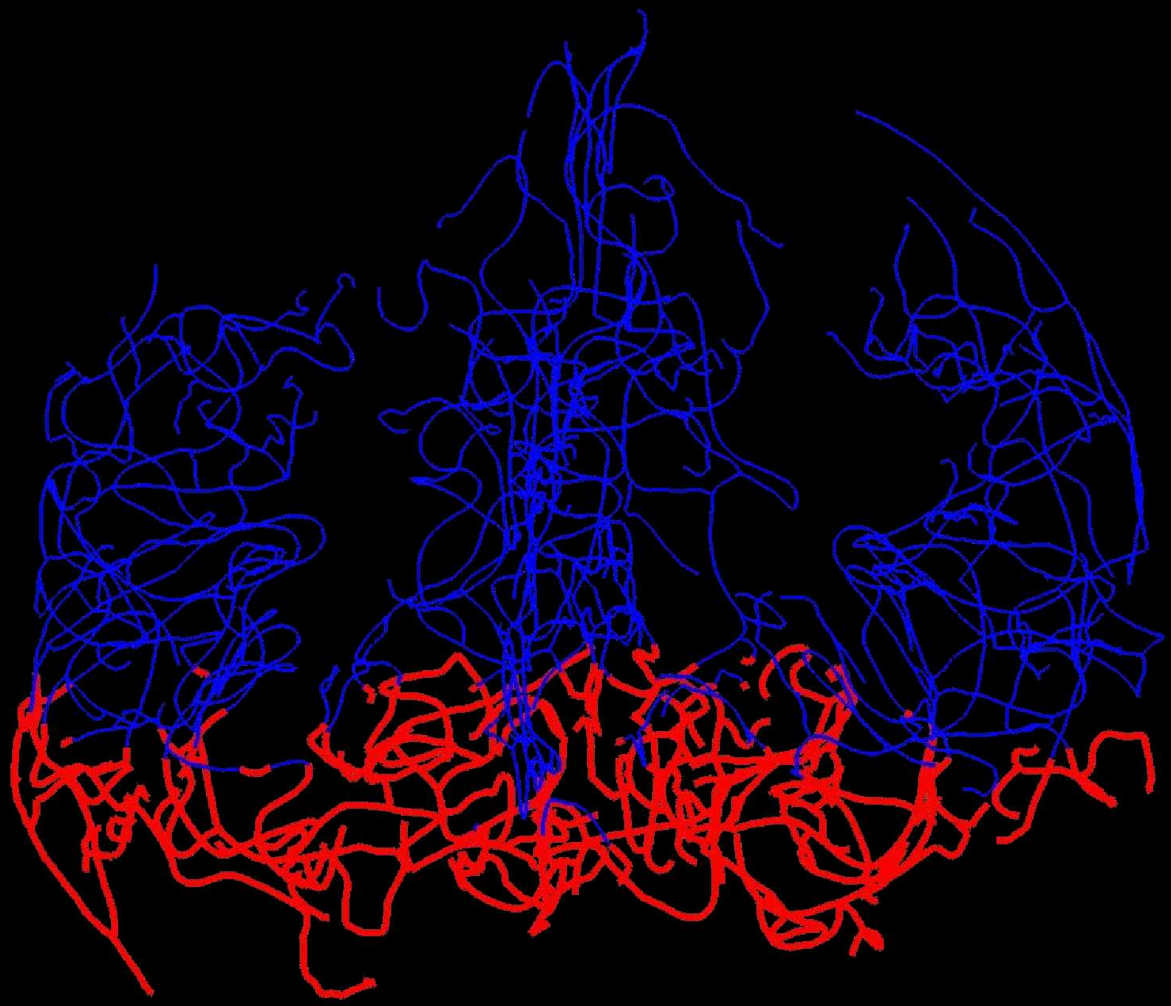

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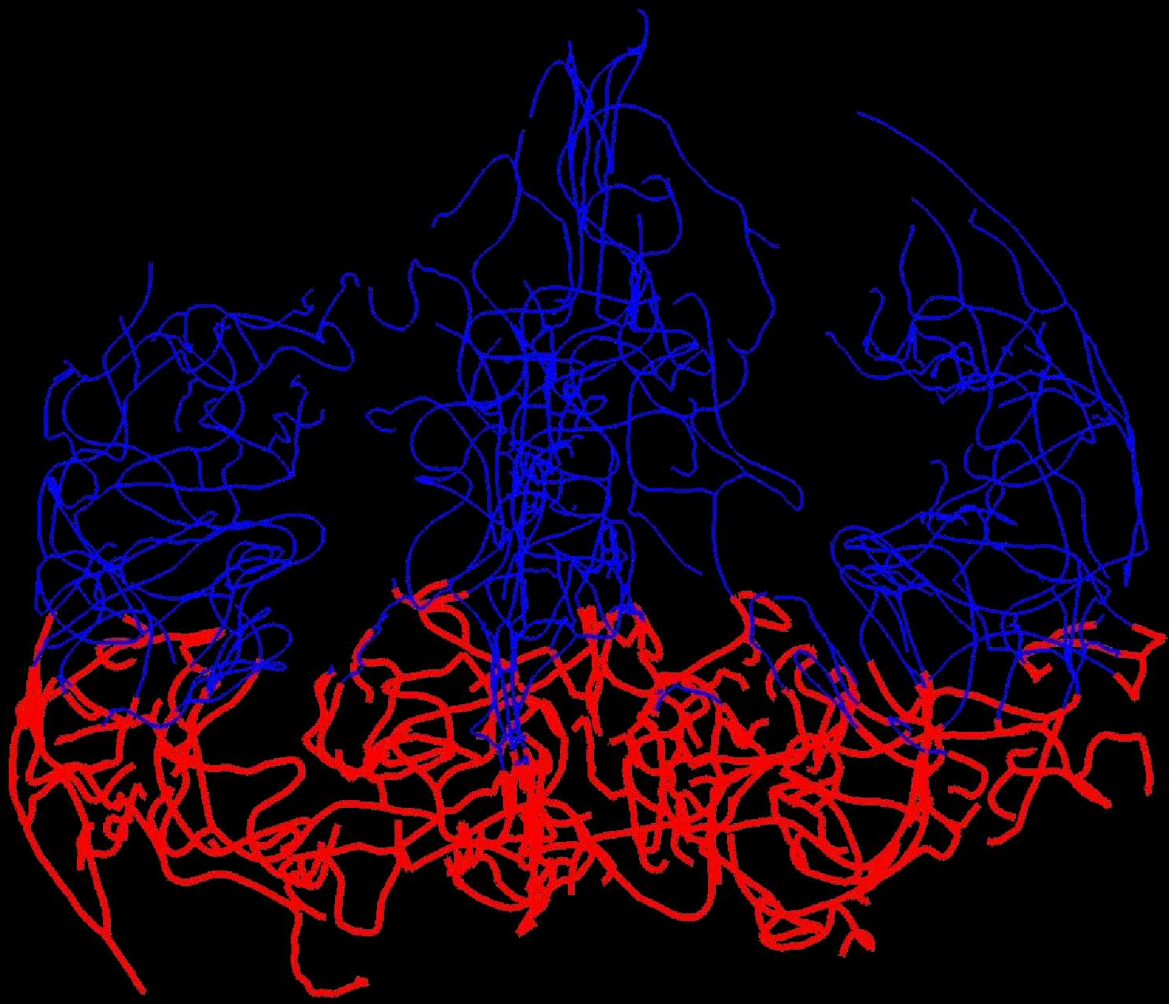

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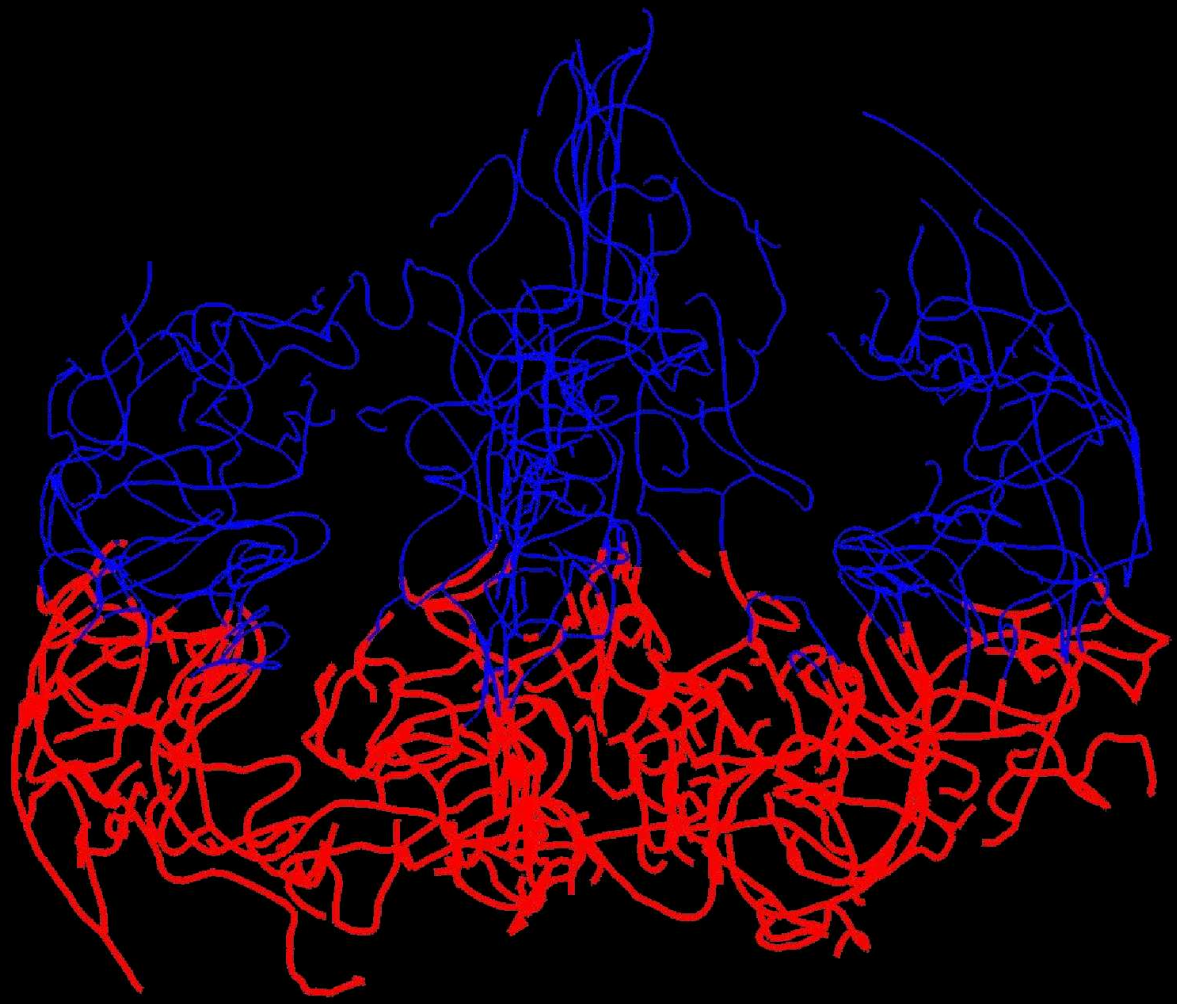

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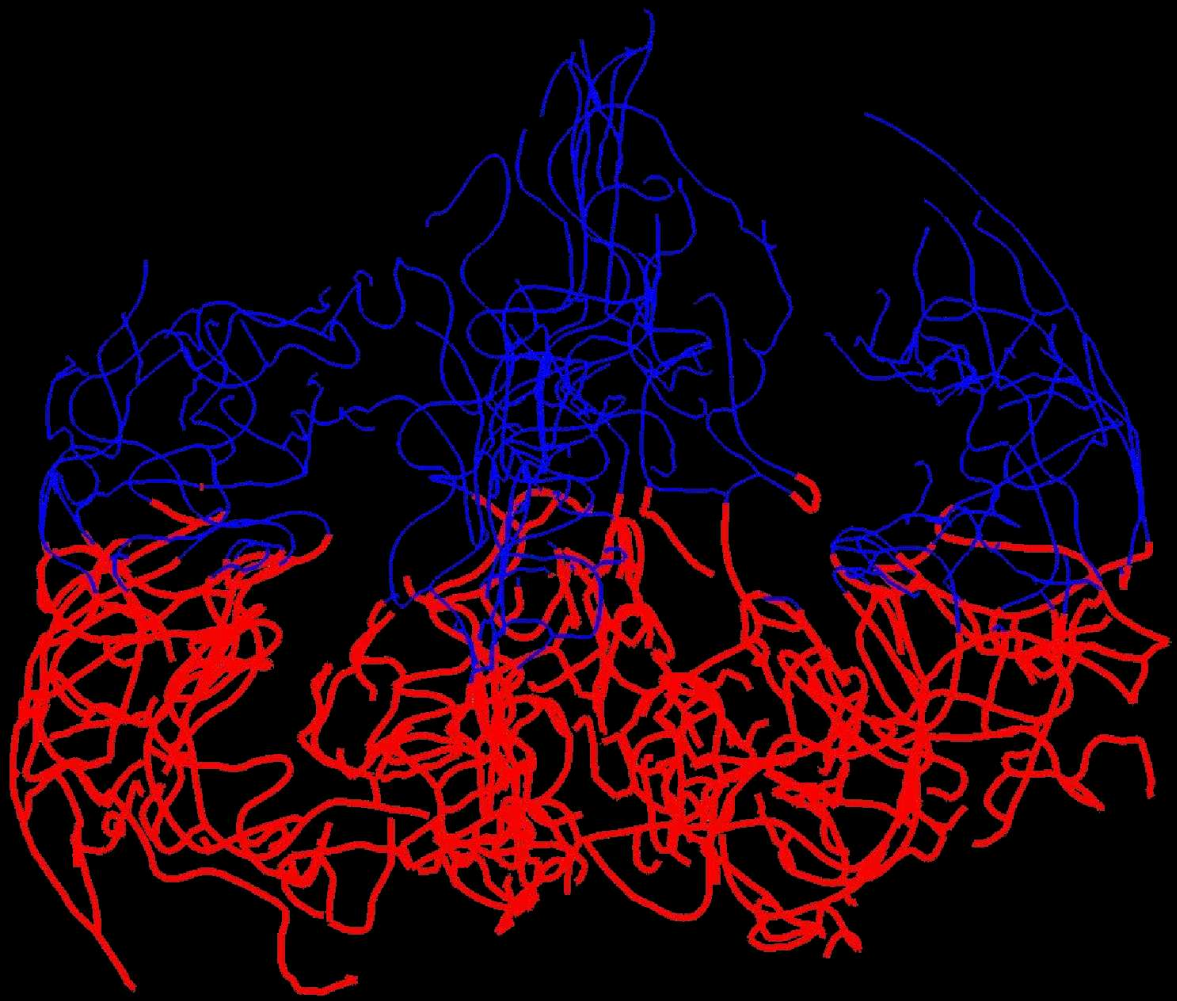

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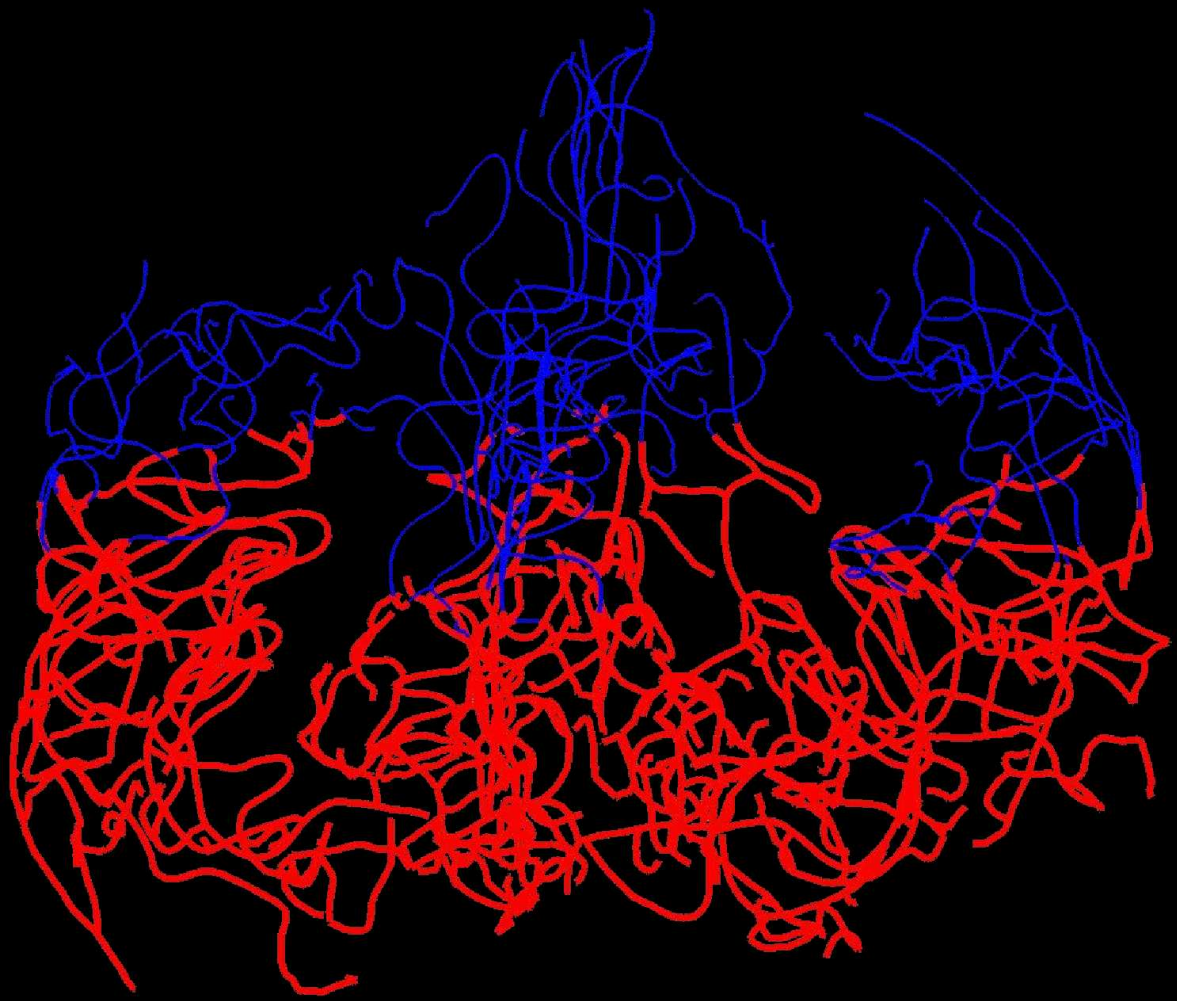

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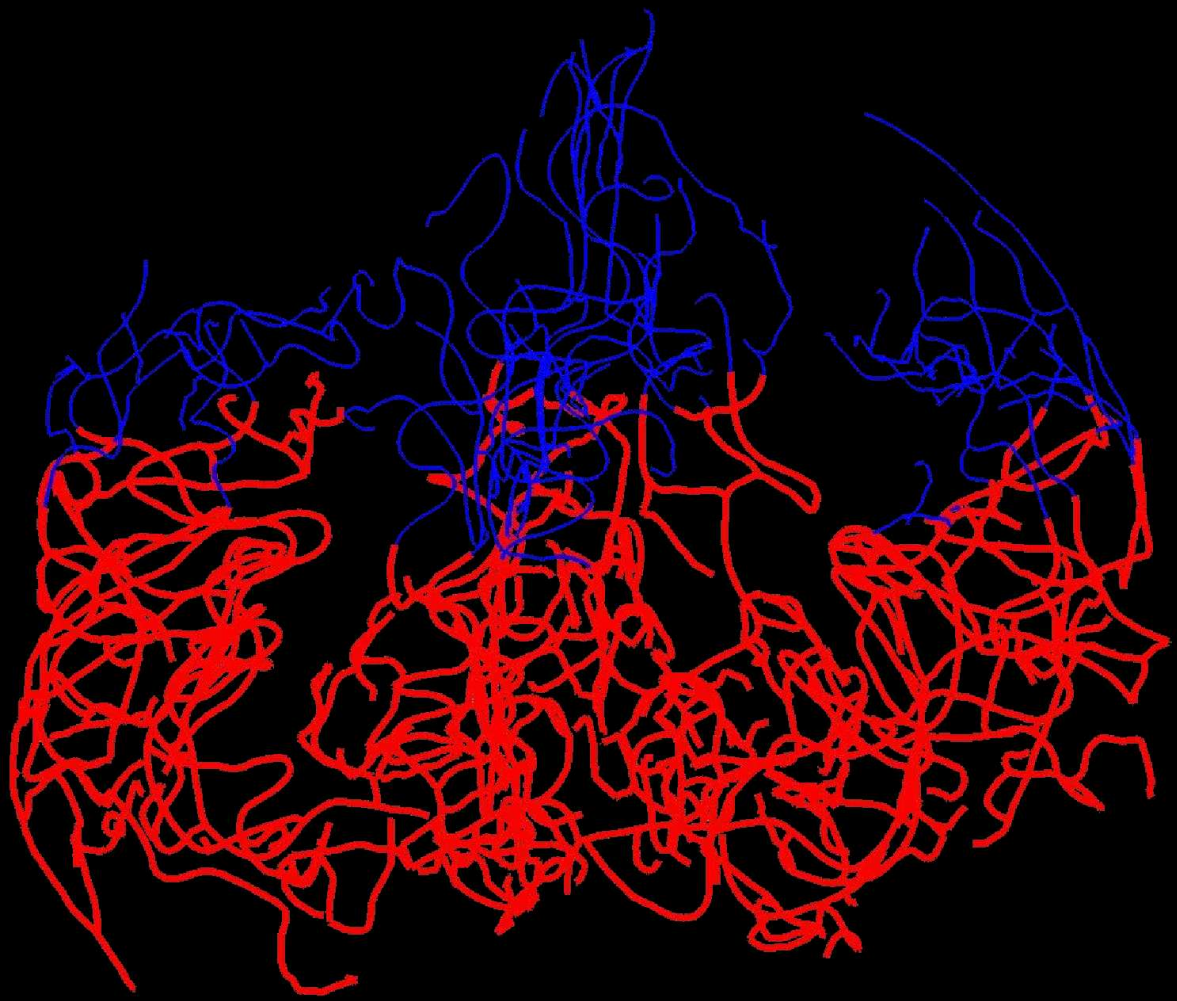

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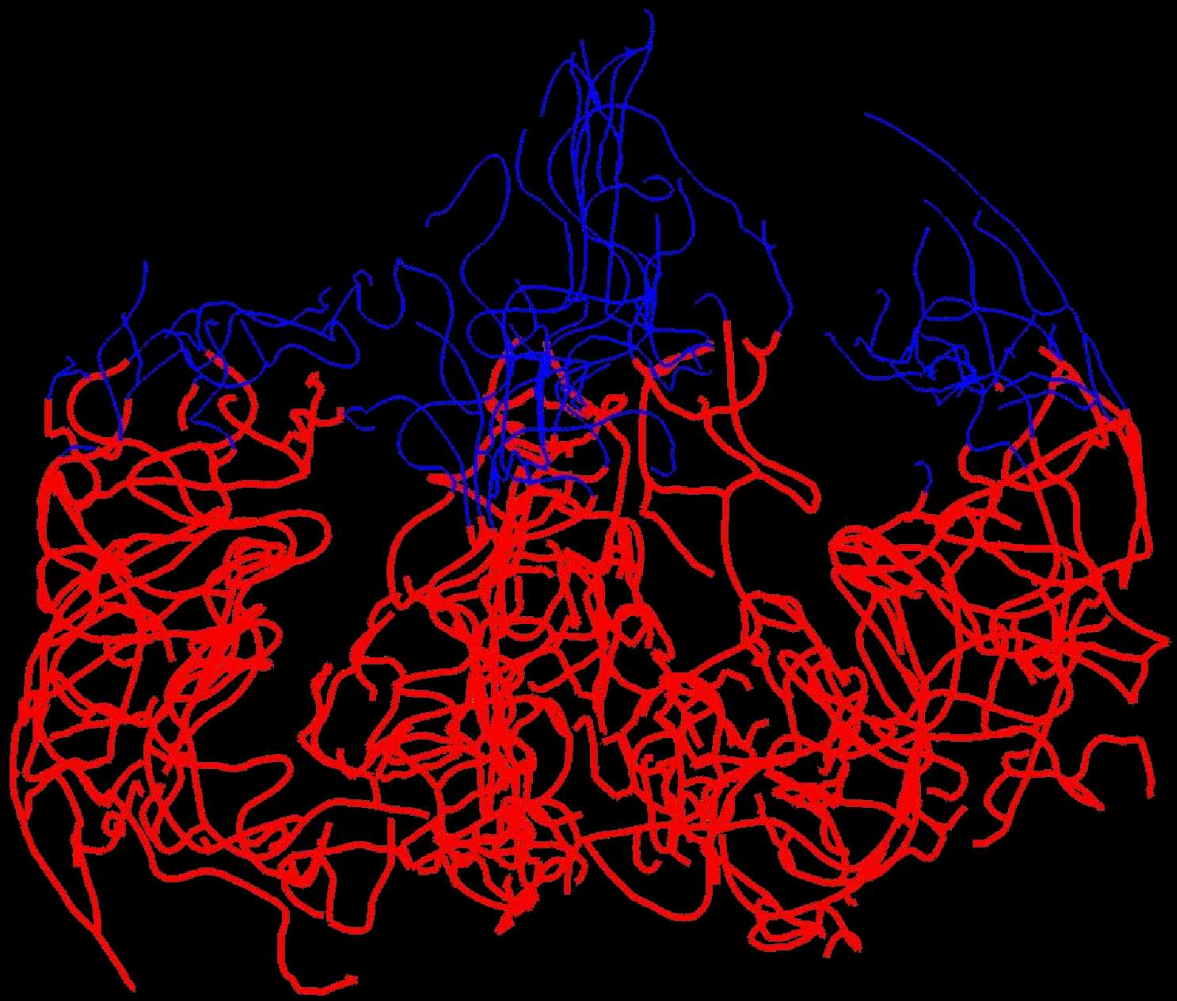

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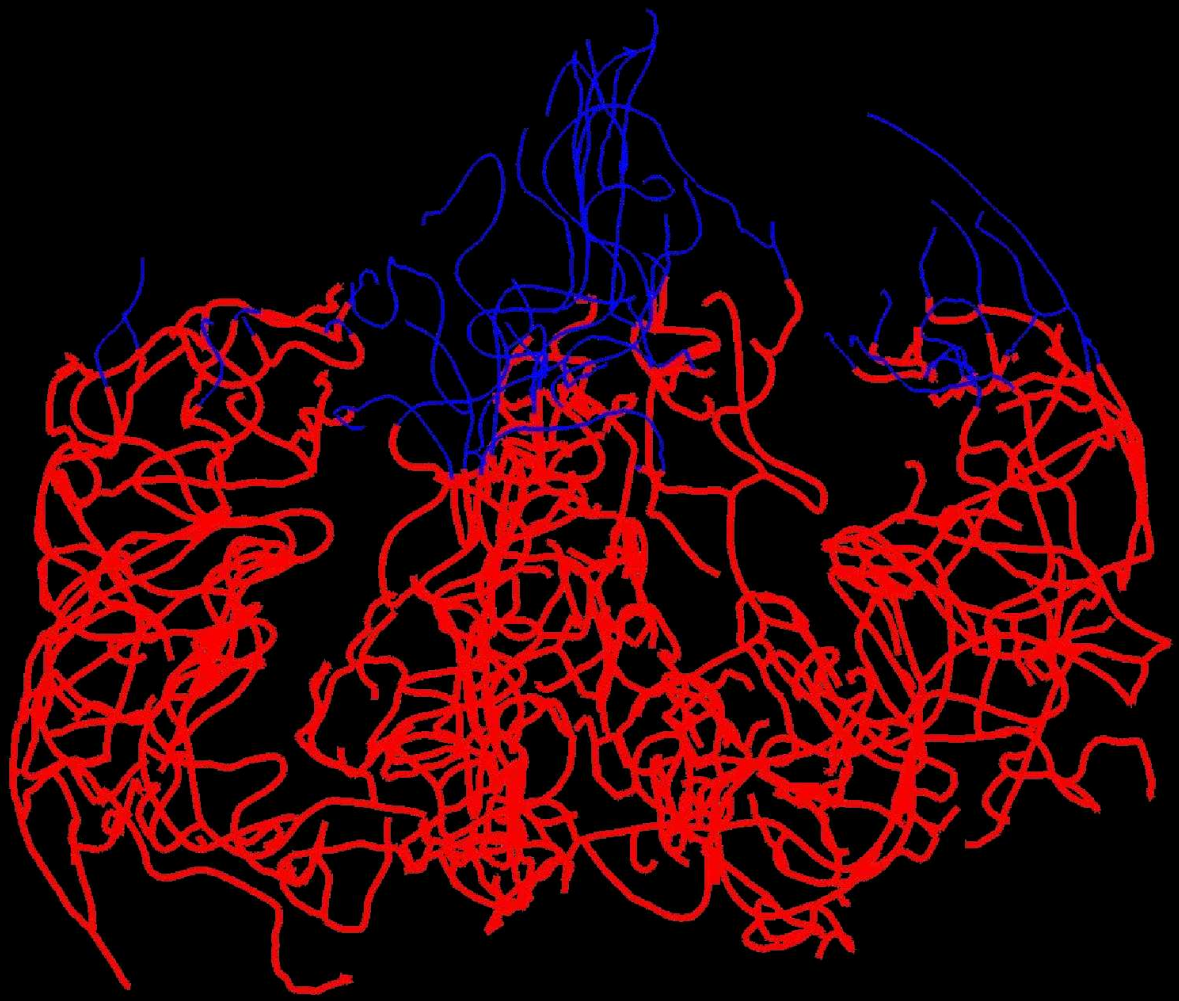

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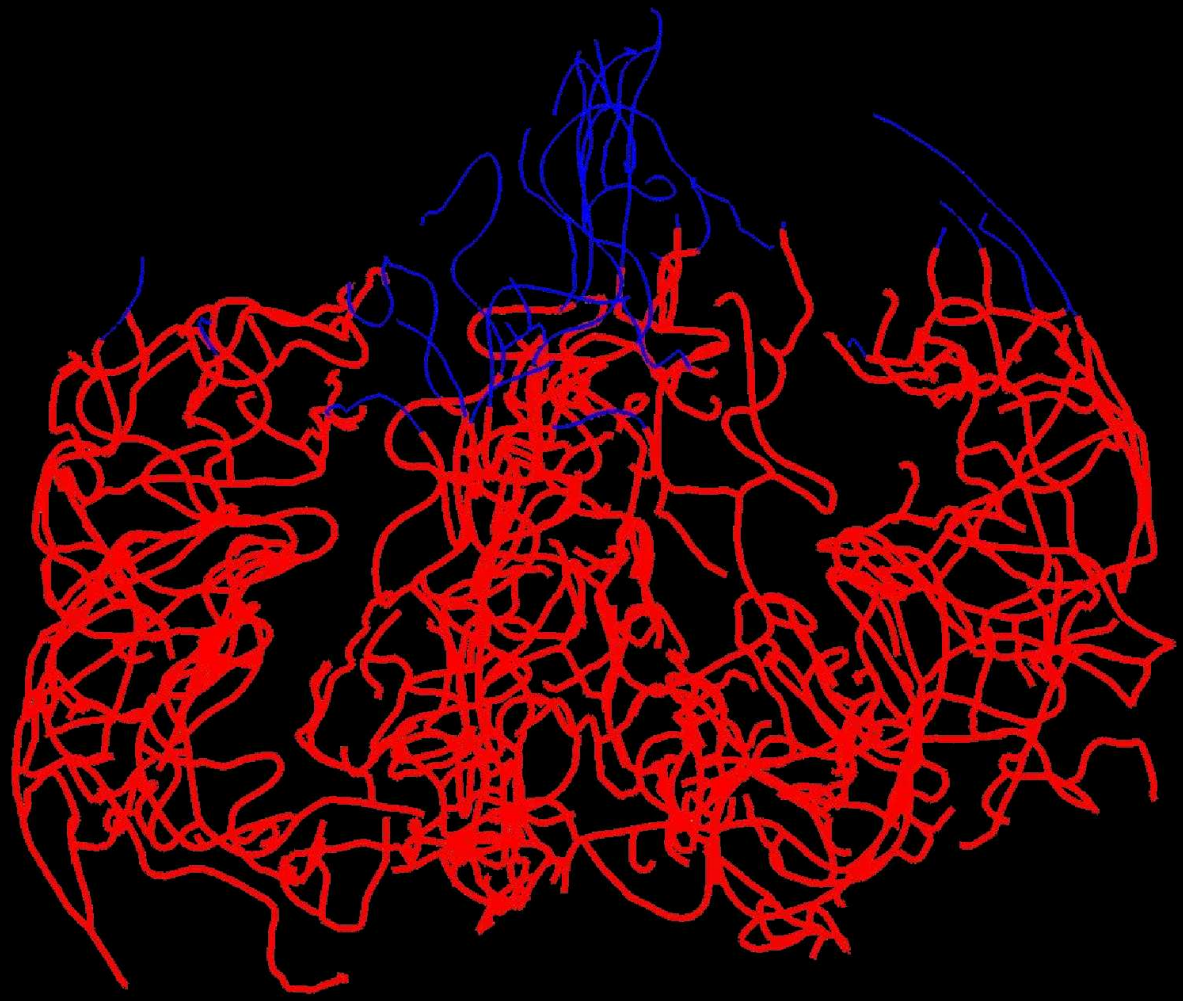

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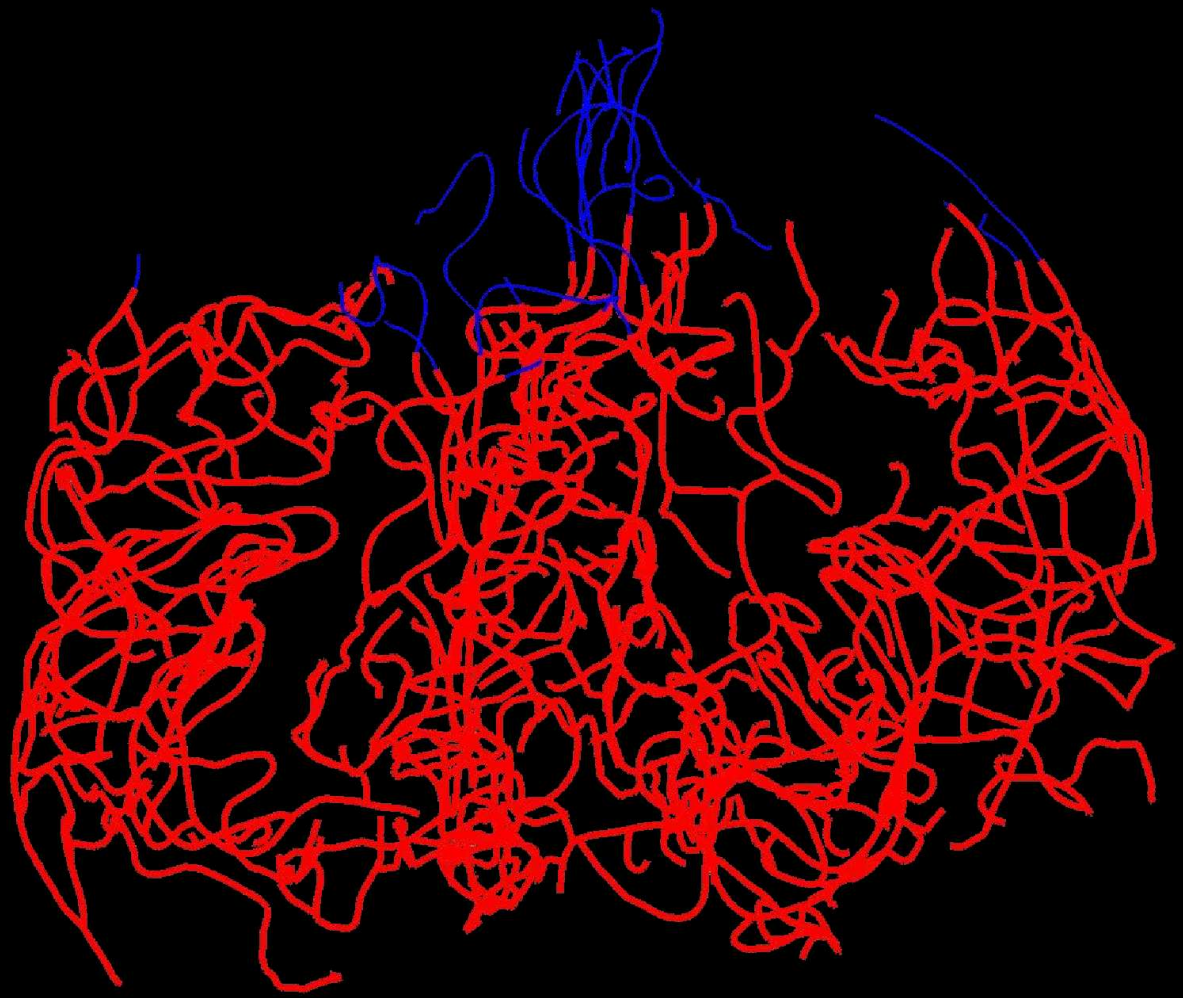

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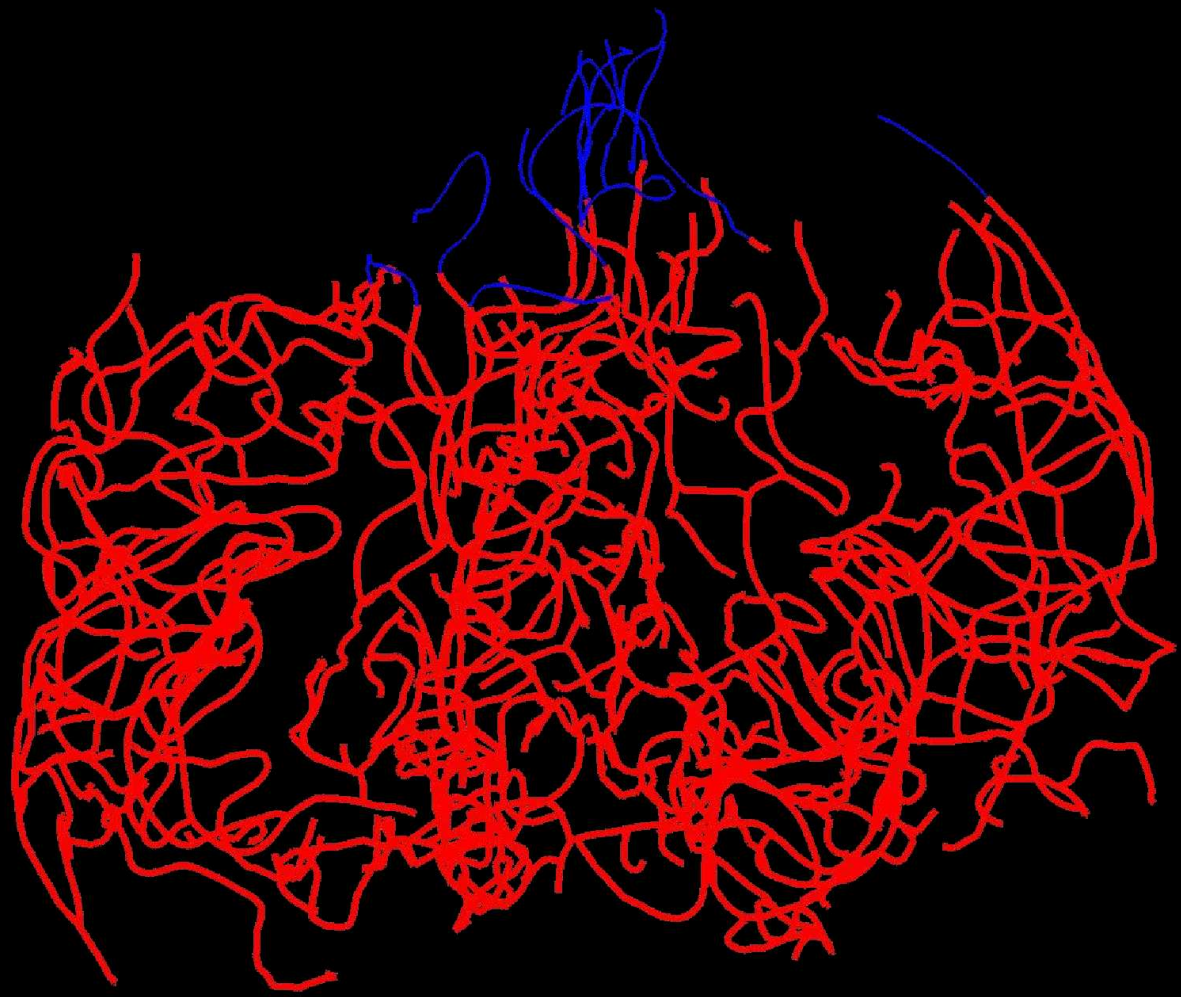

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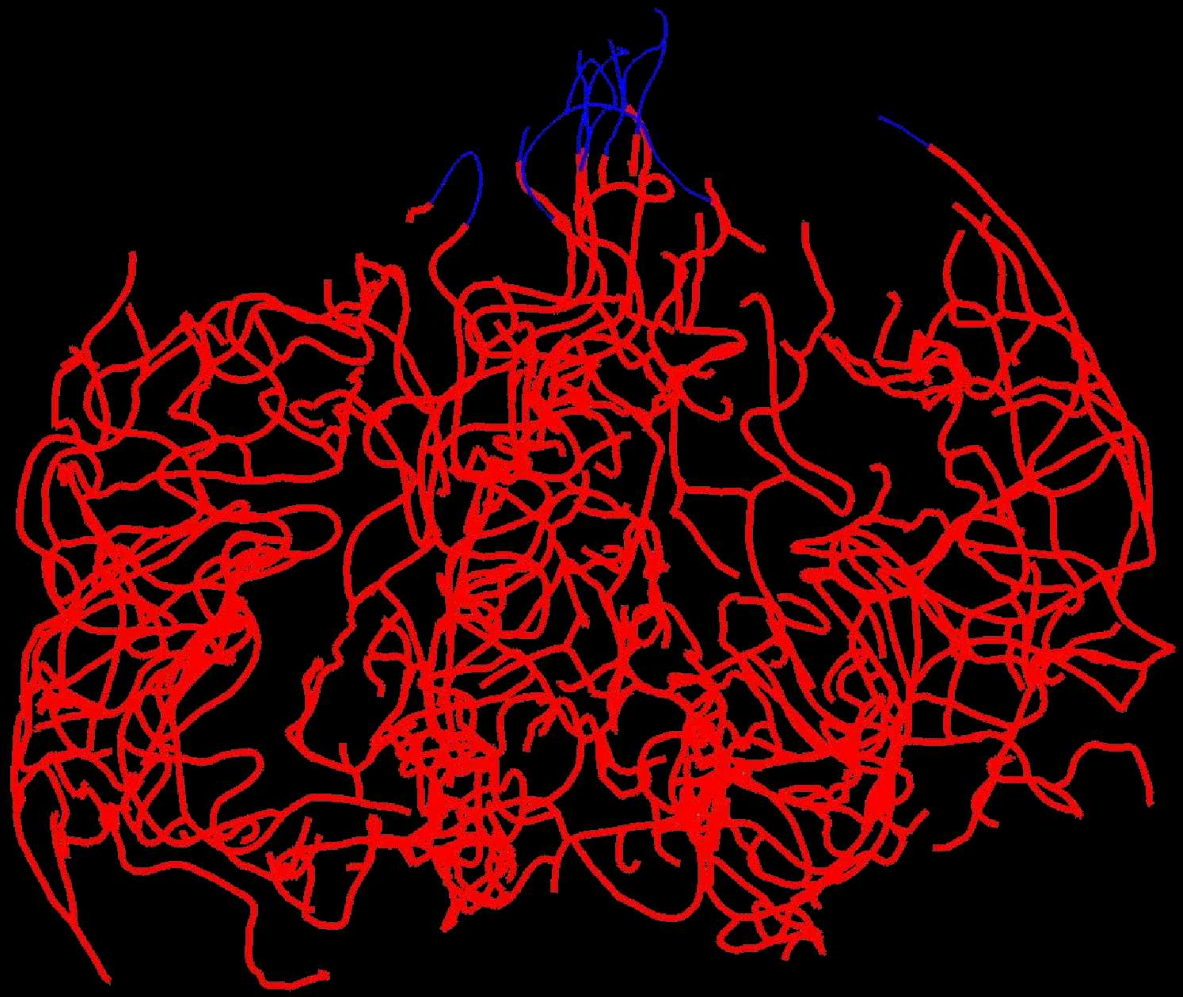

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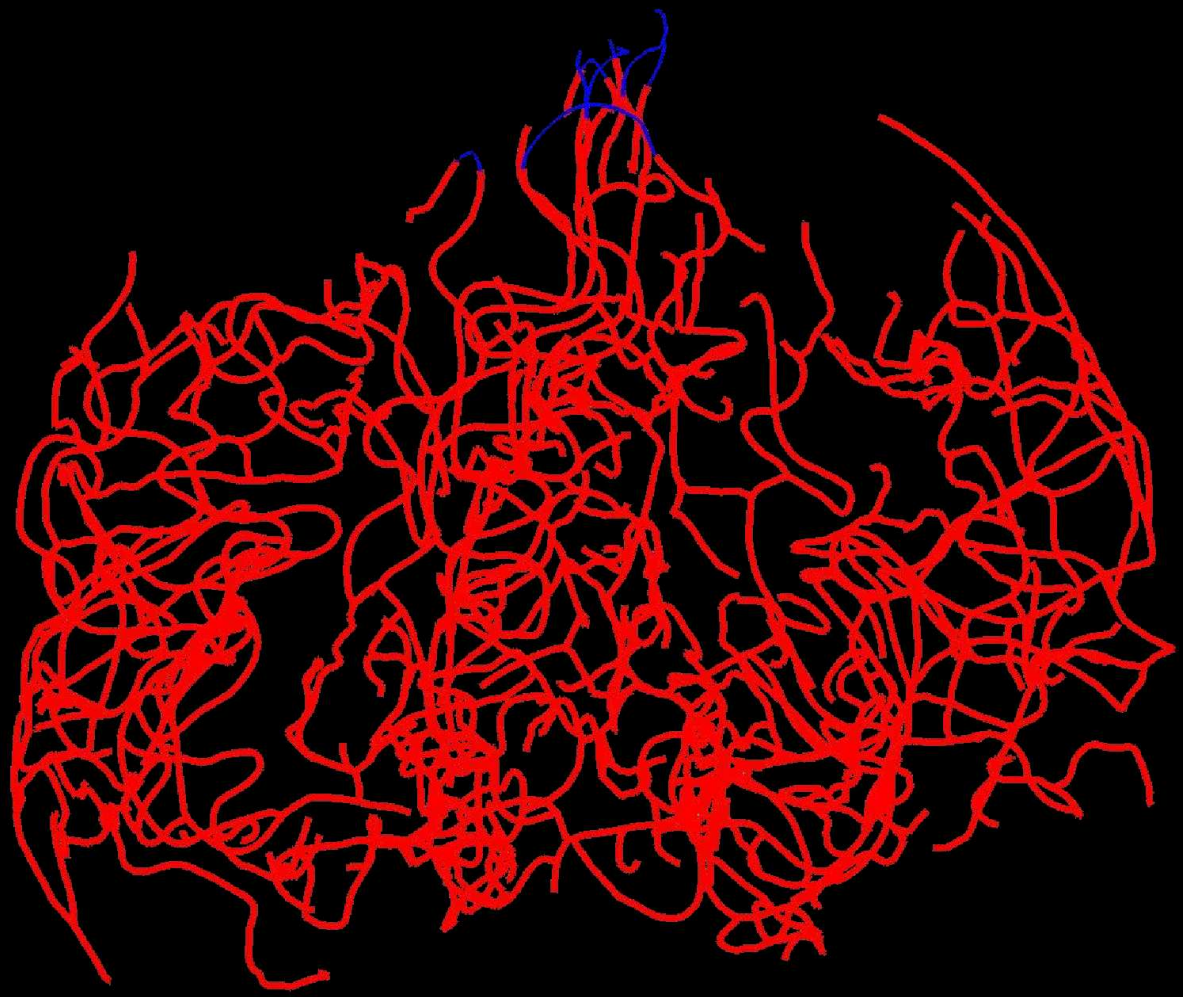

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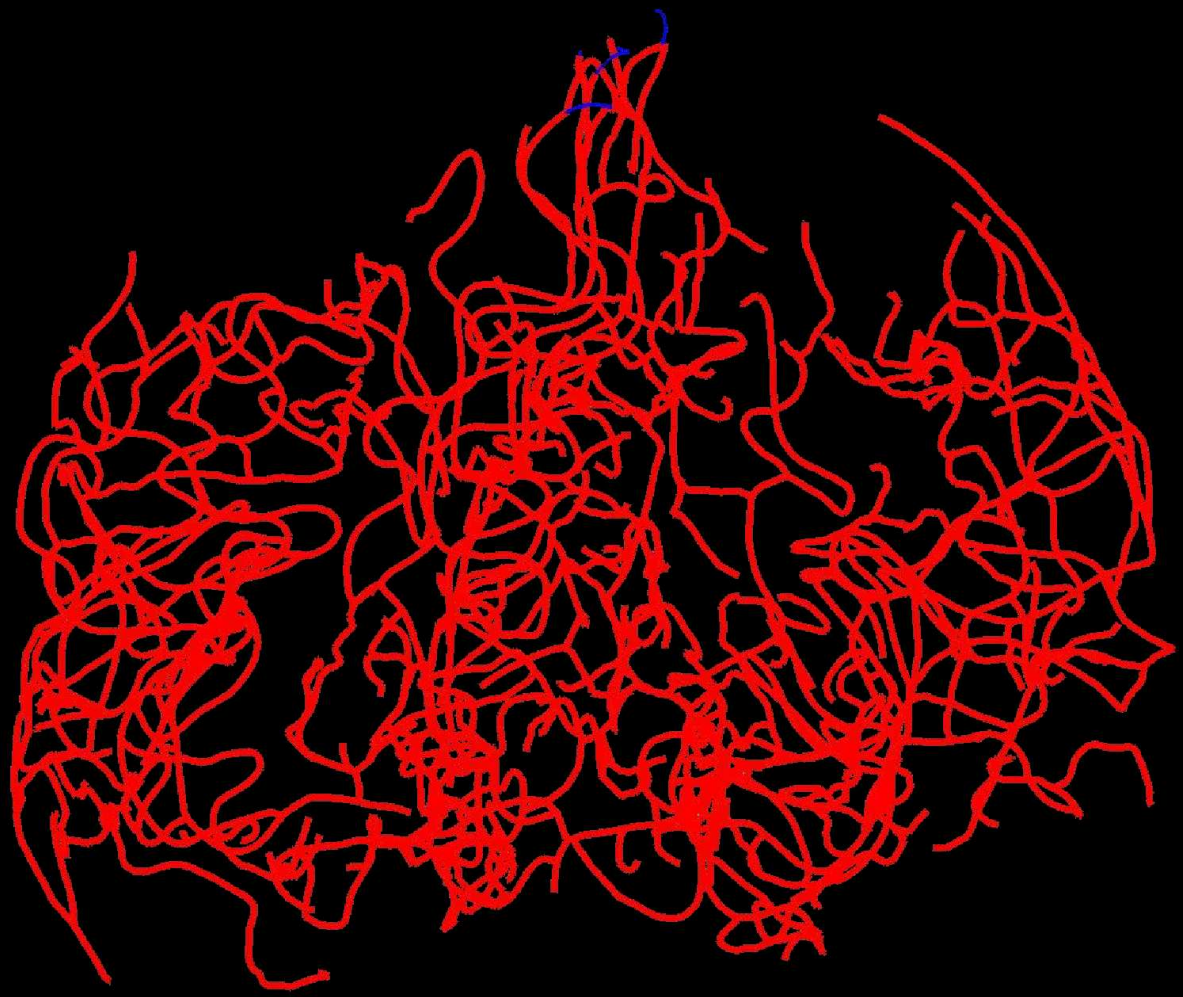

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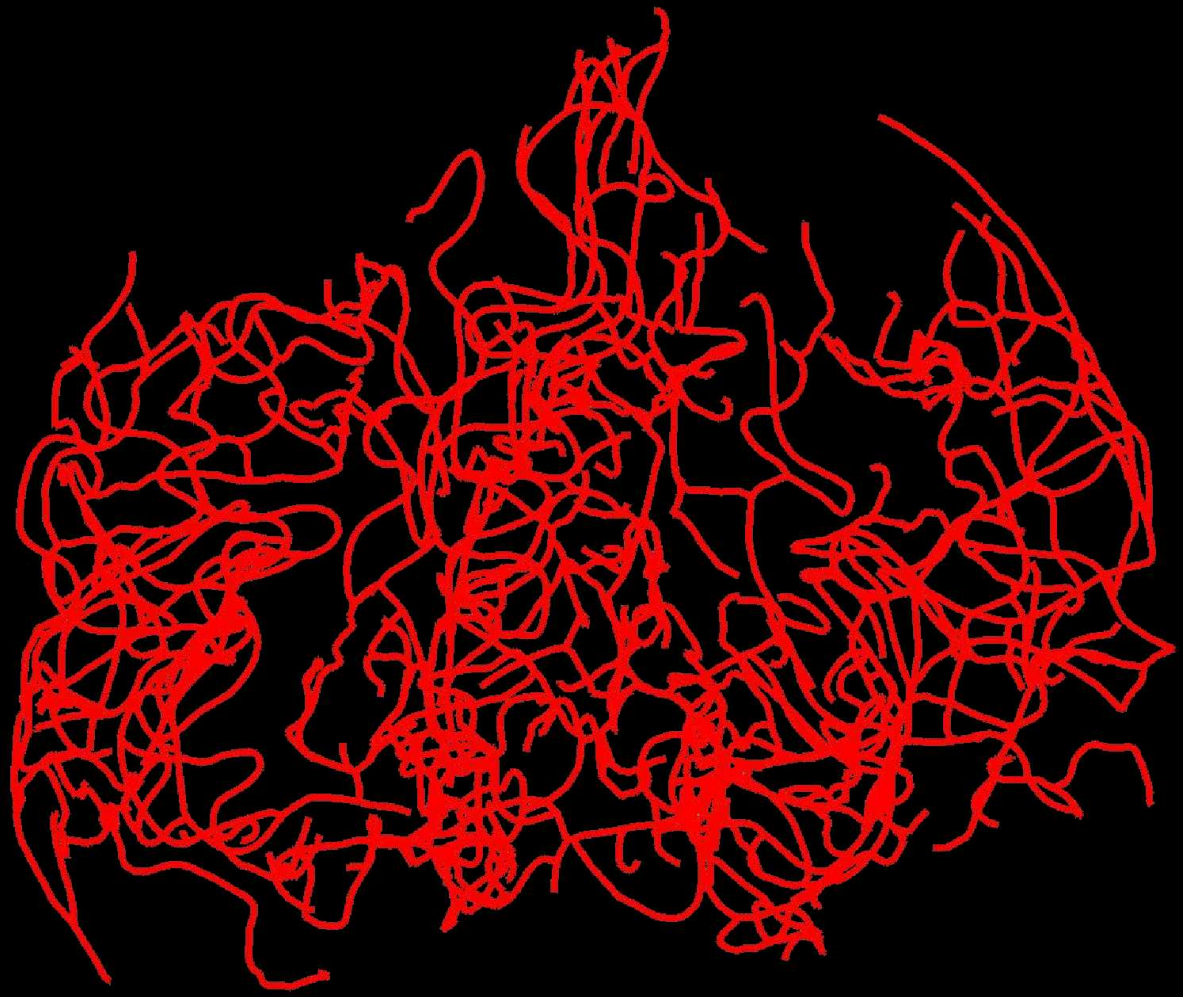

Persistent homology

Input. Topological space X filtered by set Q of subspaces: $X_q \subseteq X$ for $q \in Q$
$\Rightarrow$ Q is a partially ordered set: $X_q \subseteq X_{q'} \Leftrightarrow q \preceq q'$

Def. $\{X_q\}_{q\in Q}$ has persistent homology $\{H_q = H(X_q;\Bbbk)\}_{q\in Q}$. This is a

Def. Q-module over the poset Q:

- family $H = \{H_q\}_{q\in Q}$ of vector spaces over the field $\Bbbk$ with
- homomorphism $H_q \to H_{q'}$ whenever $q \prec q'$ in Q such that
- $H_q \to H_{q''}$ equals the composite $H_q \to H_{q'} \to H_{q''}$ whenever $q \prec q' \prec q''$

Examples

- points in $\mathbb{R}^n$: $Q = \{0,\dots,m\}$ or $\mathbb{R}$ 1-parameter ("ordinary") persistence
- brain arteries: $Q = \{0,\dots,m\}$ or $\mathbb{R}$ 1-parameter ("ordinary") persistence
- wing veins: $Q = \mathbb{Z}^2$ or $\mathbb{R}^2$ 2 discrete or continuous parameters
- probability distributions: $Q = \mathbb{R}^2$ 2 continuous parameters
- $Q = \mathbb{Z}^n \Leftrightarrow H = \mathbb{Z}^n$-graded $\Bbbk[x_1,\dots,x_n]$-module
- $Q = \mathbb{R}^n \Leftrightarrow H = \mathbb{R}^n$-graded $\Bbbk[\mathbb{R}^n_+]$-module

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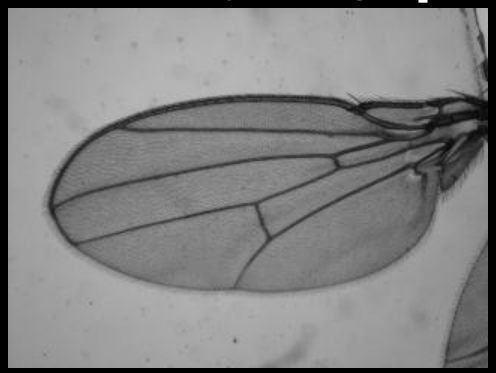
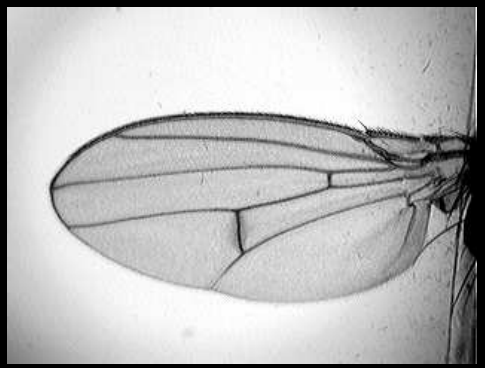
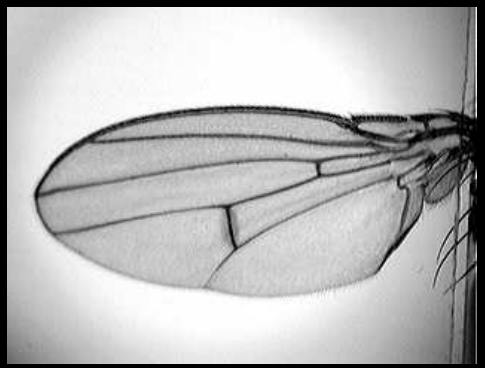
Fruit fly wings

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

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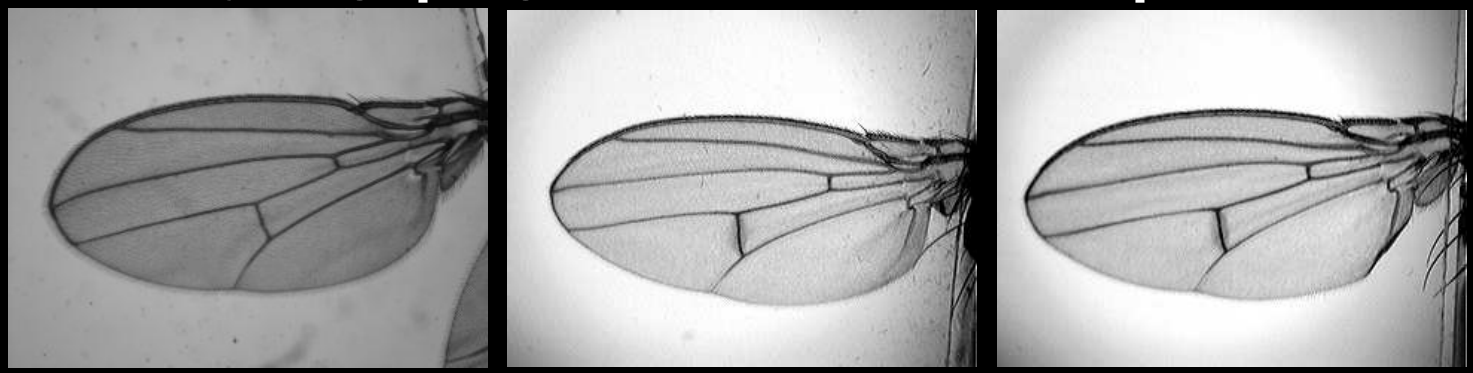
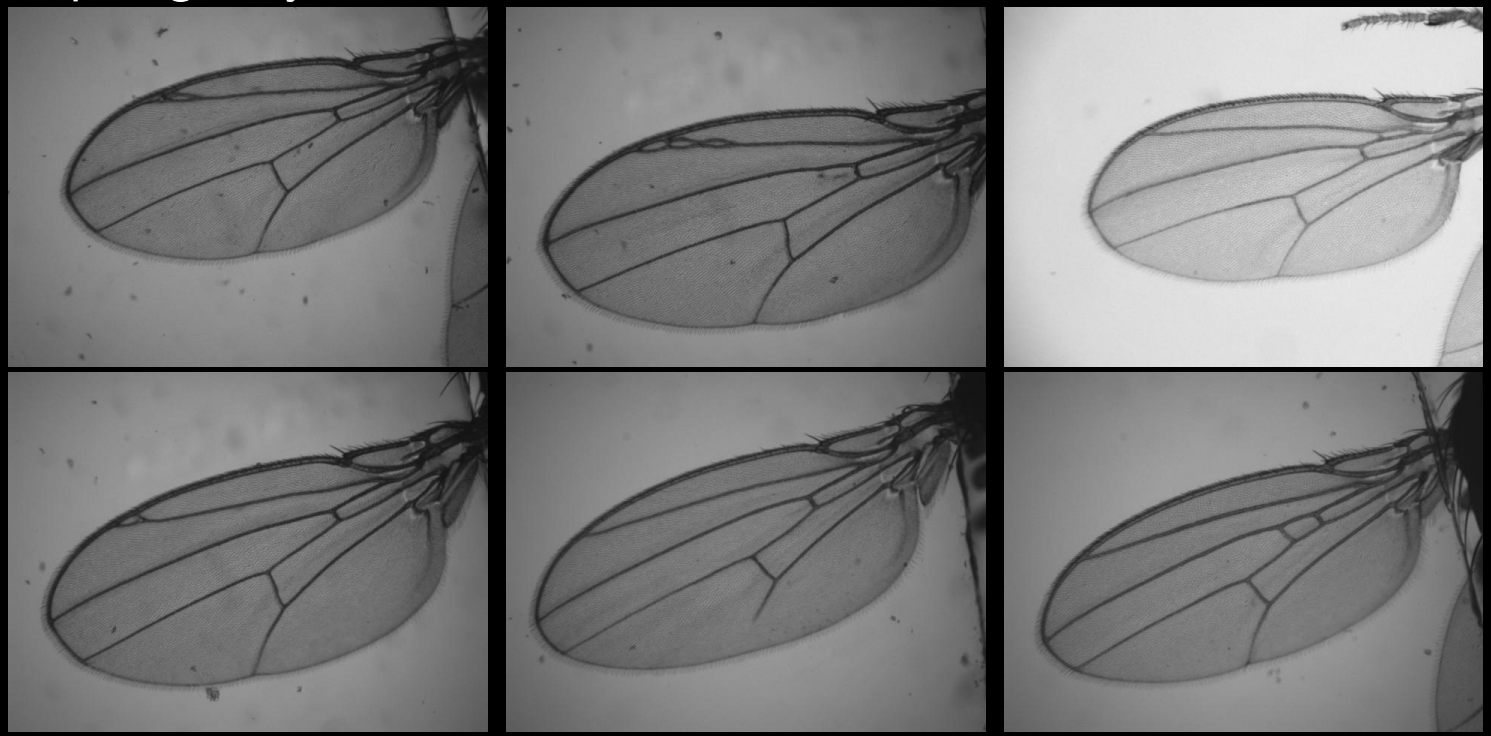
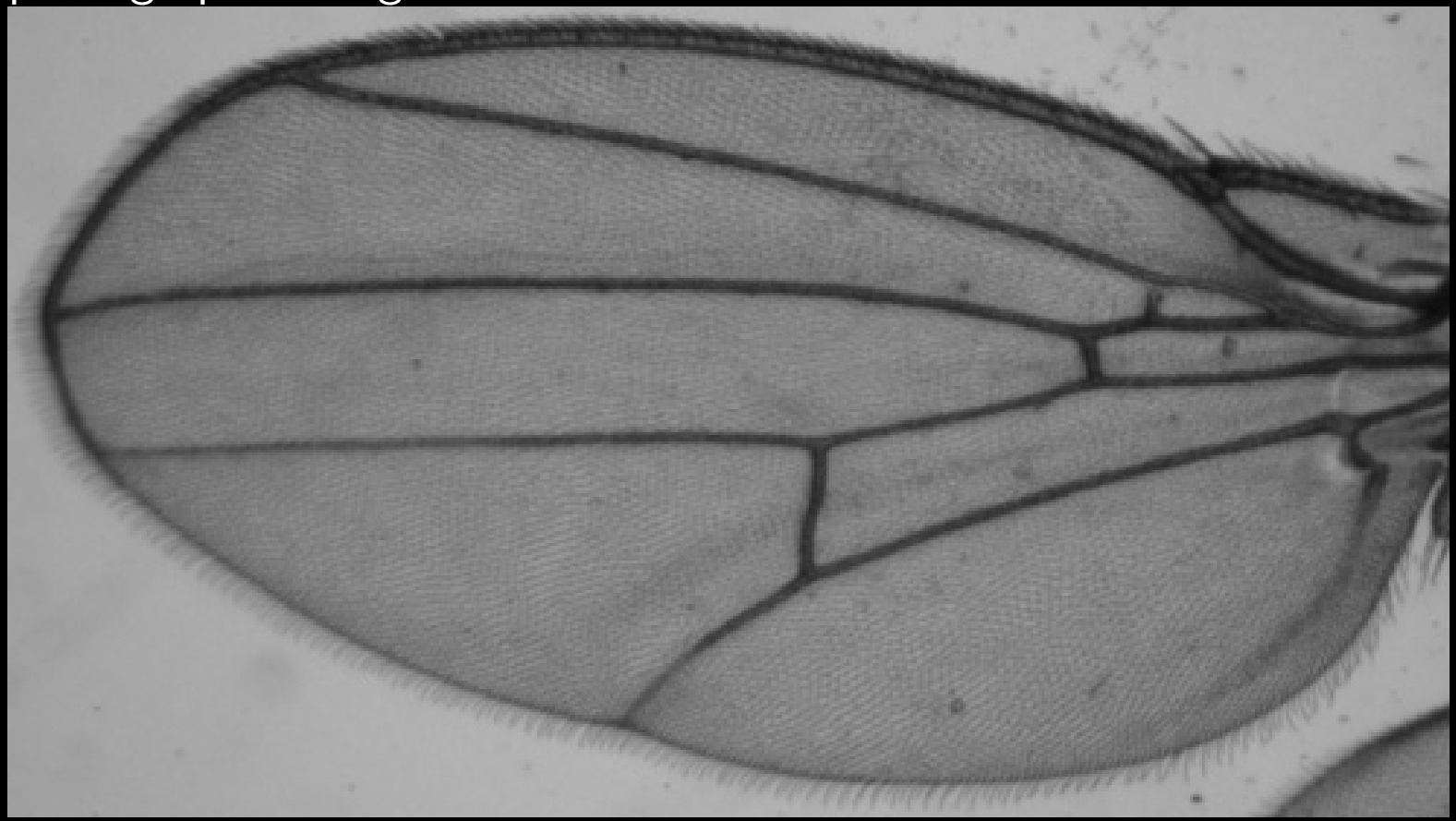


Topologically abnormal veins:



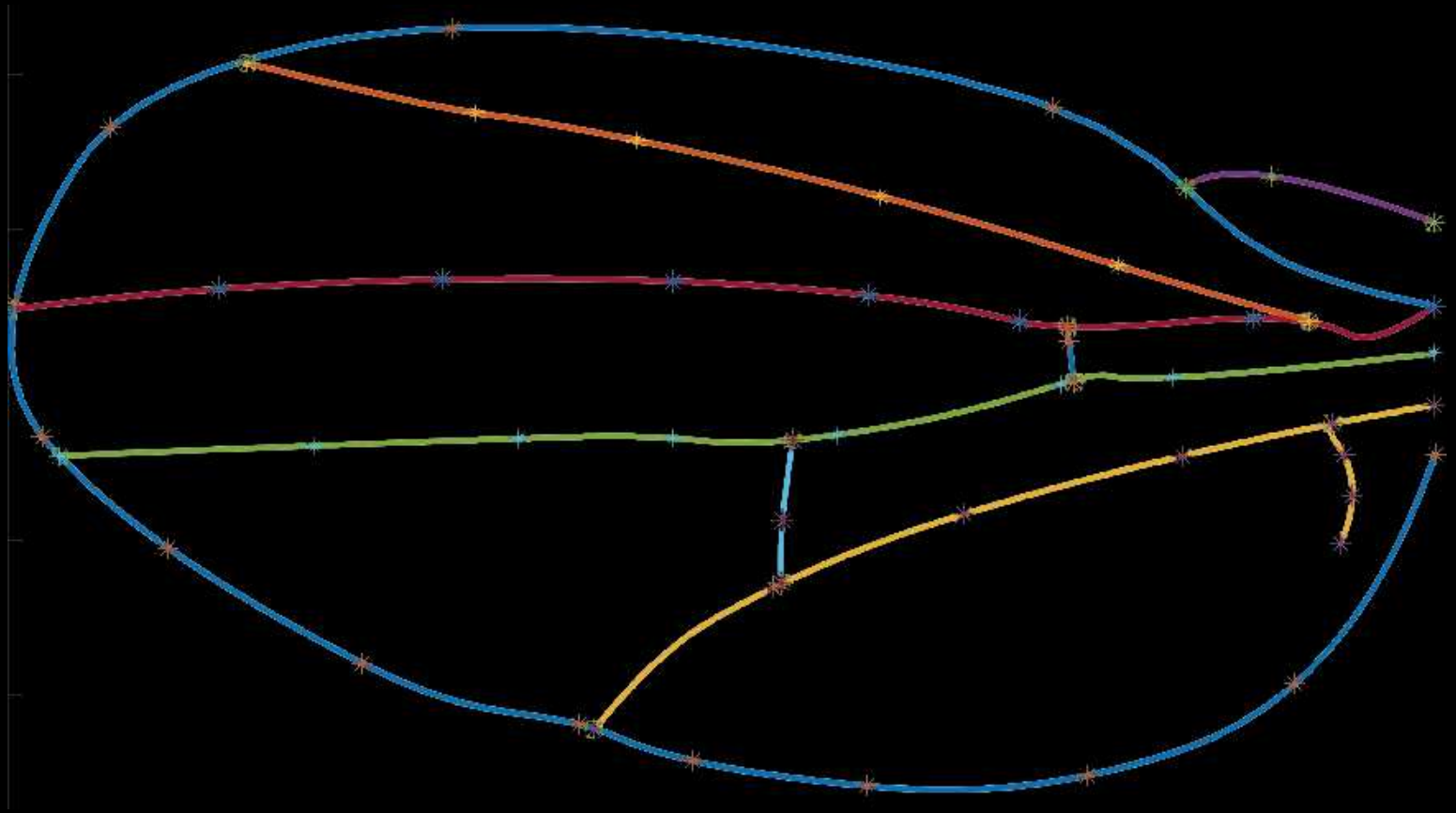
Fruit fly wings

photographic image



Fruit fly wings

spline



Biological background

What generates topological novelty?

[Houle, et al.]: selecting for certain continuous wing vein deformations yields

- skew toward more oddly shaped wings, but also
- much higher rate of topological novelty

Hypothesis. Topological novelty arises when directional selection pushes continuous variation in a developmental program beyond a certain threshold.

Test the hypothesis

- "plot" wings in "form space"
- determine whether topological variants lie "in the direction of" continuous shape selected for, and at the extreme in that direction

Goal. Statistical analysis encompassing topological vein variation, giving appropriate weight to new singular points in addition to varying shape

- compare phenotypic distance to genotypic distance; needs
- metric specifying distance between topologically distinct wings

To proceed. Statistics with fly wings as data objects $\rightsquigarrow$ statistics with multiparameter persistence diagrams as data objects

Need. Data structures, algorithms, theoretical guarantees

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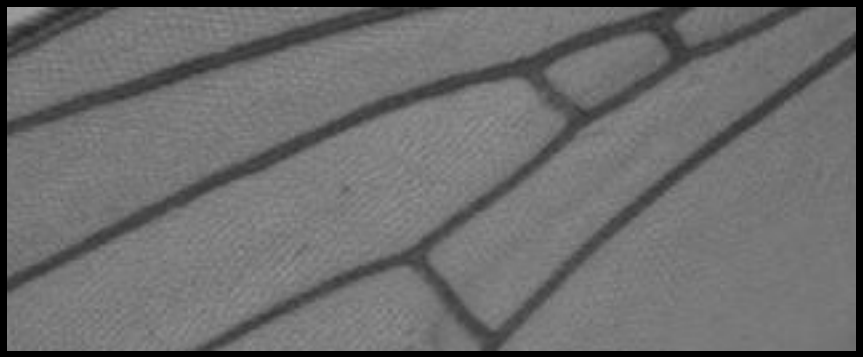
Wing vein persistence [w/Houle, et al., ongoing]

Example. Encode fruit fly wing with 2-parameter persistence

- 1st parameter: distance from vertex set
- 2nd parameter: distance from edge set



Sublevel set $W_{r,s}$ is near edges but far from vertices $\Rightarrow H_{r,s} = H_i(W_{r,s})$

Wing vein persistence [w/Houle, et al., ongoing]

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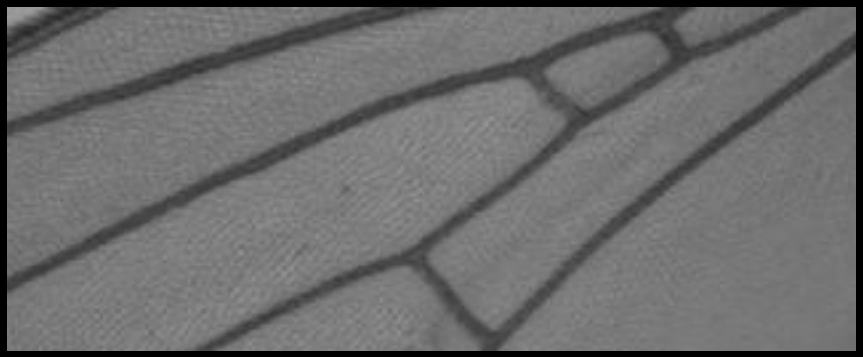

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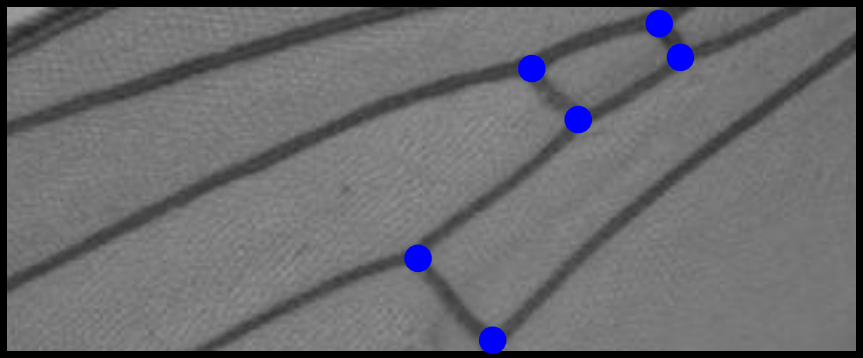

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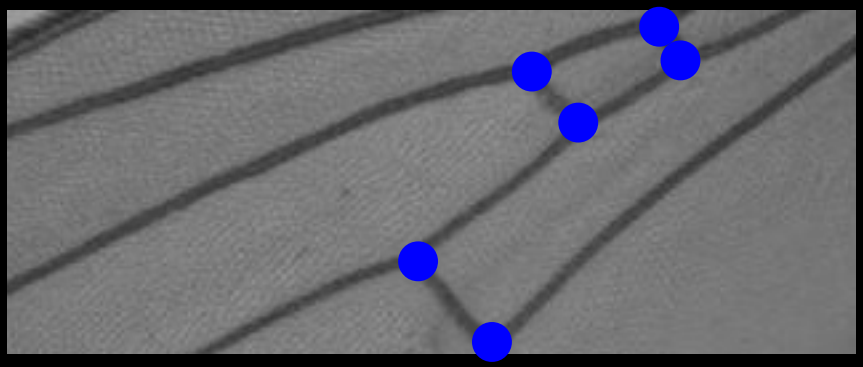

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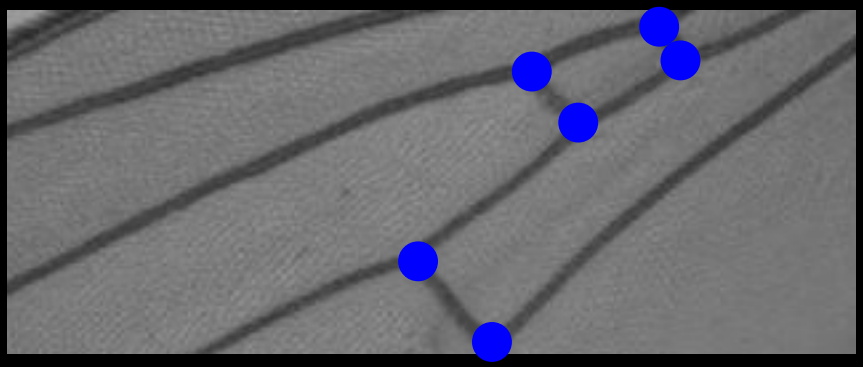
Example. Encode fruit fly wing with 2-parameter persistence

- 1st parameter: distance from vertex set given as points in $\mathbb{R}^2$
- 2nd parameter: distance from edge set given as Bézier curves



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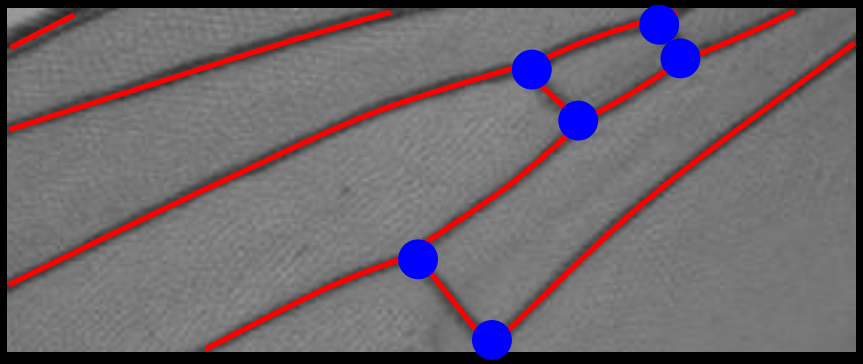

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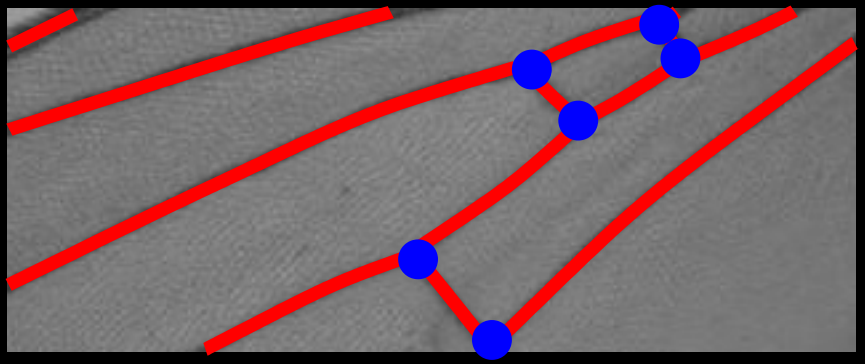

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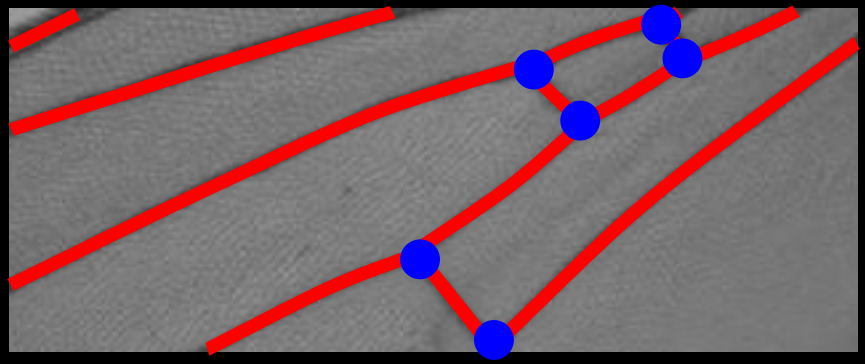
Wing vein persistence [w/Houle, et al., ongoing]

Example. Encode fruit fly wing with 2-parameter persistence

- 1st parameter: distance from vertex set (require distance $\geq -r$)
- 2nd parameter: distance from edge set given as Bézier curves



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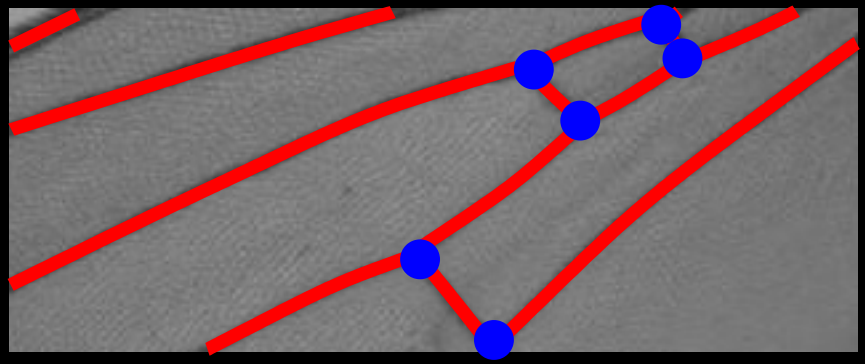

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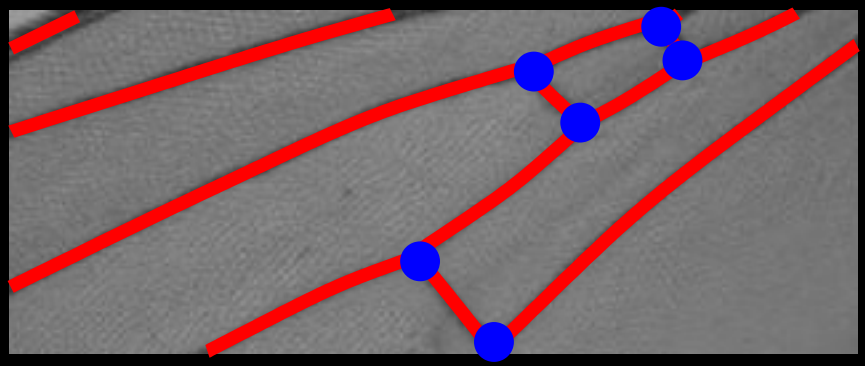

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Wing vein persistence [w/Houle, et al., ongoing]

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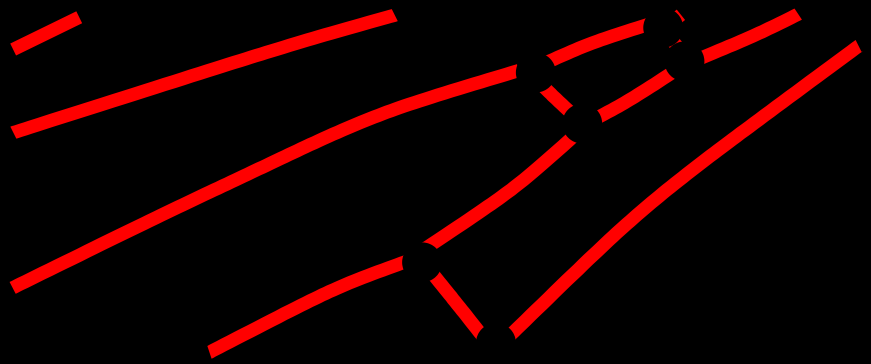

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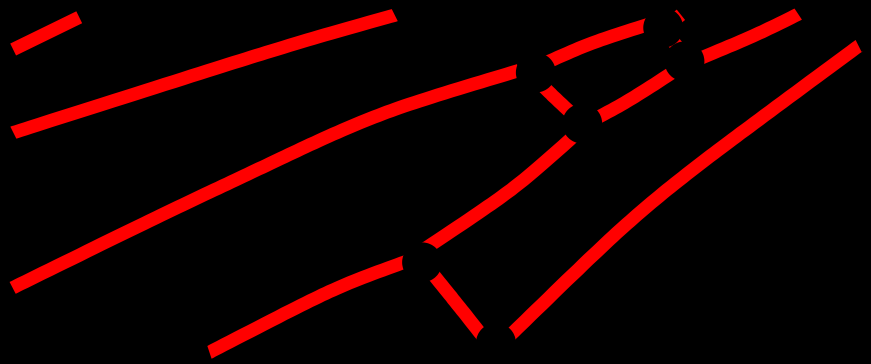

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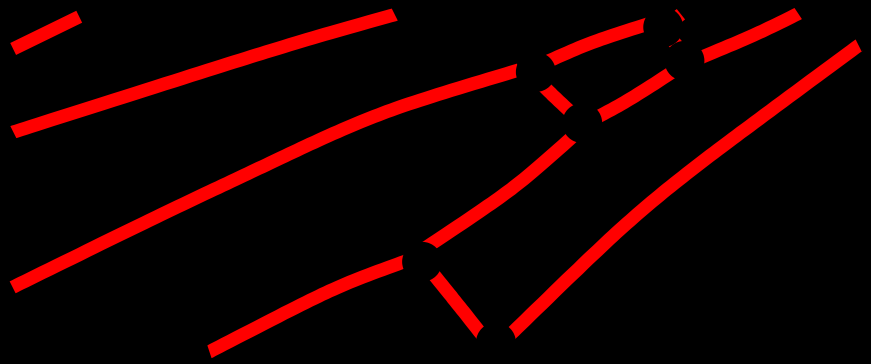

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Multiscale summary

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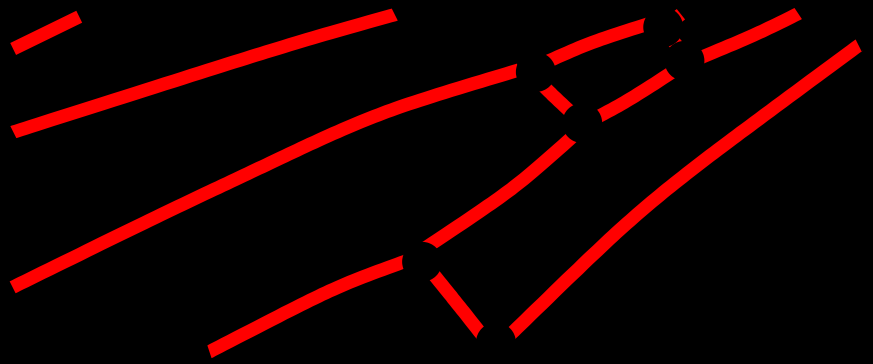

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Multiscale summary

$\mathbb{Z}^2$-module:

$$\begin{array}{ccccccc}
 & & \uparrow & & \uparrow & & \uparrow & \\
 & \to & H_{r-\varepsilon,s+\delta} & \to & H_{r,s+\delta} & \to & H_{r+\varepsilon,s+\delta} & \to \\
 & & \uparrow & & \uparrow & & \uparrow & \\
 & \to & H_{r-\varepsilon,s} & \to & H_{r,s} & \to & H_{r+\varepsilon,s} & \to \\
 & & \uparrow & & \uparrow & & \uparrow & \\
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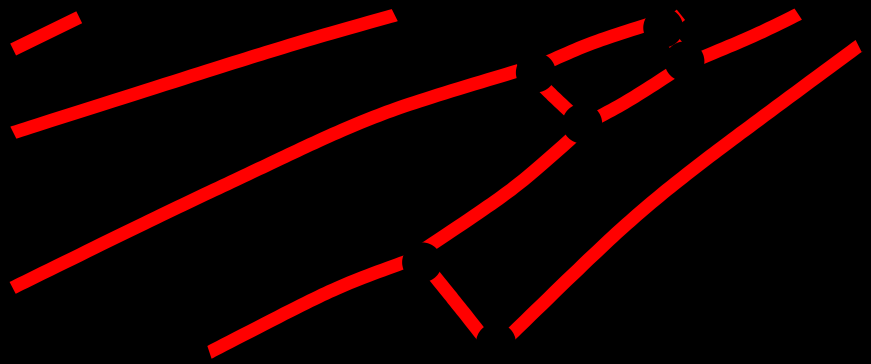

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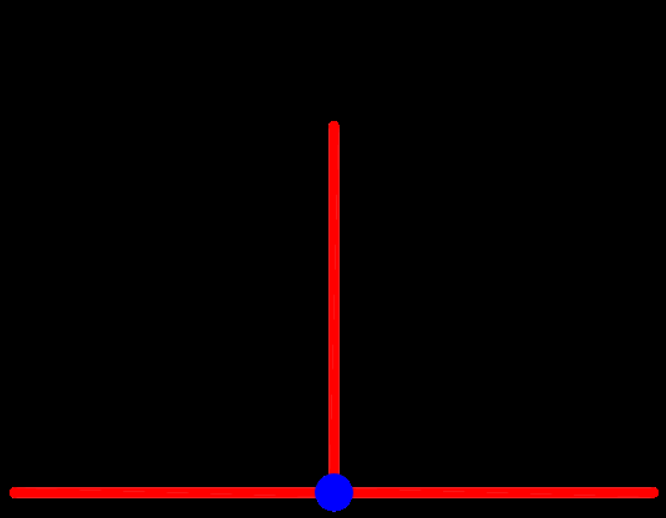

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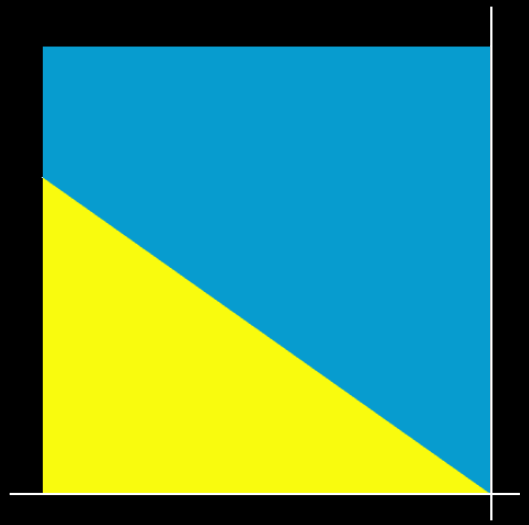

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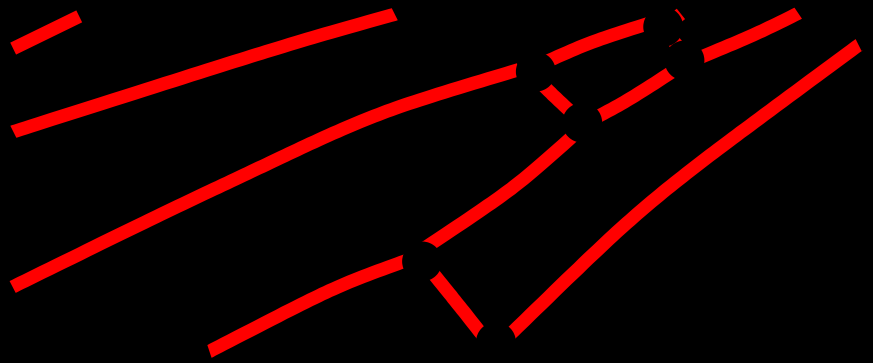

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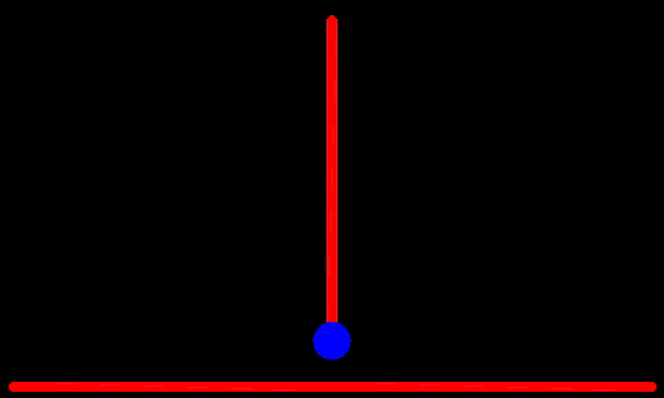

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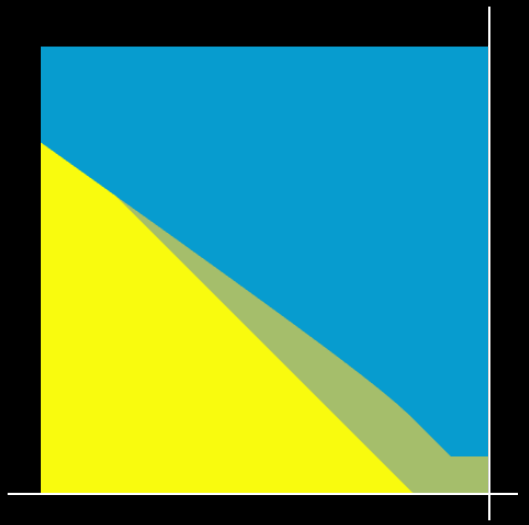

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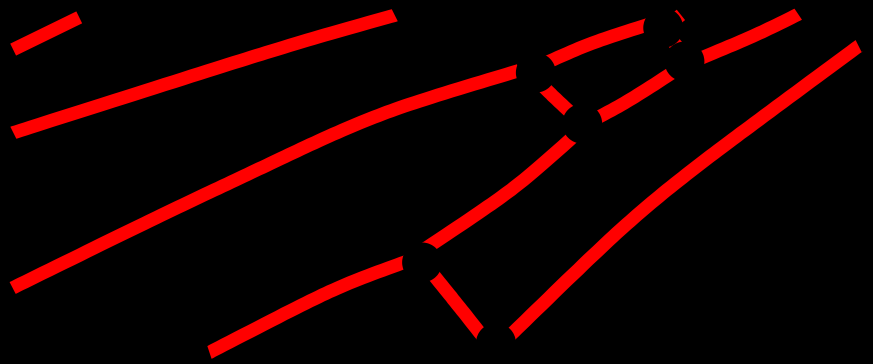

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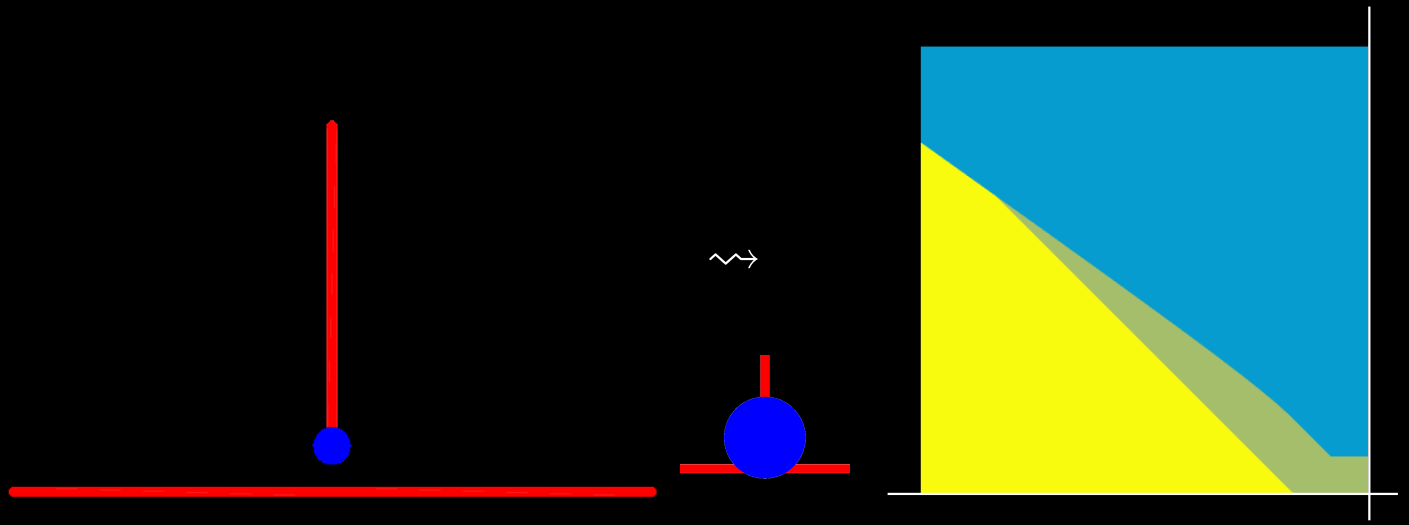

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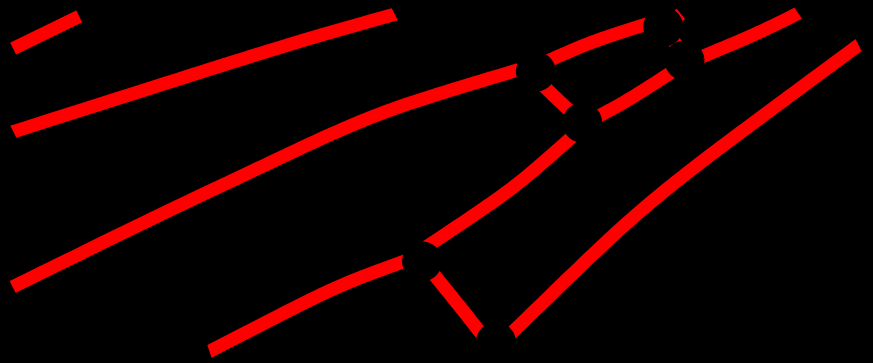

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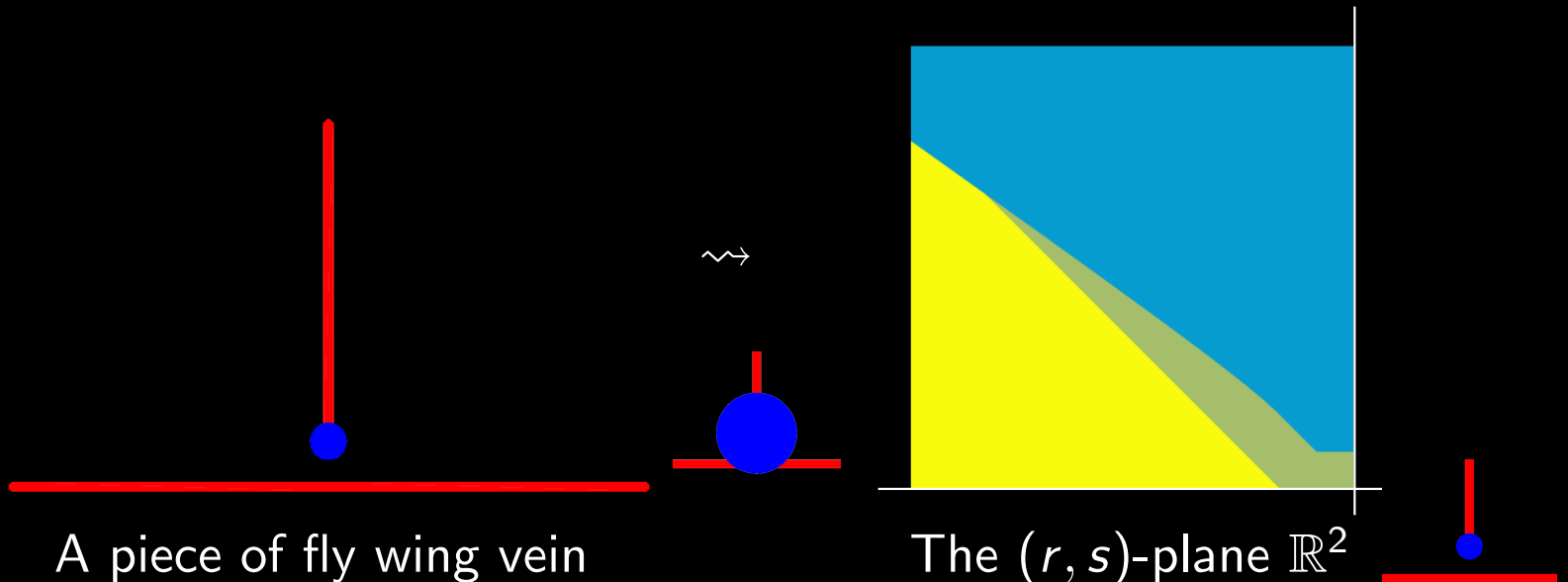

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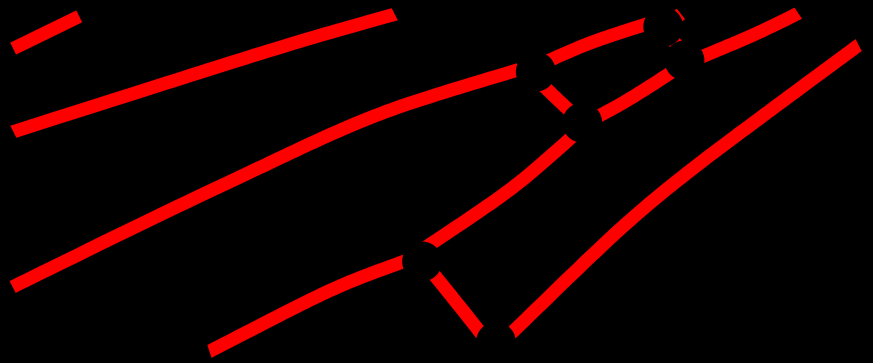

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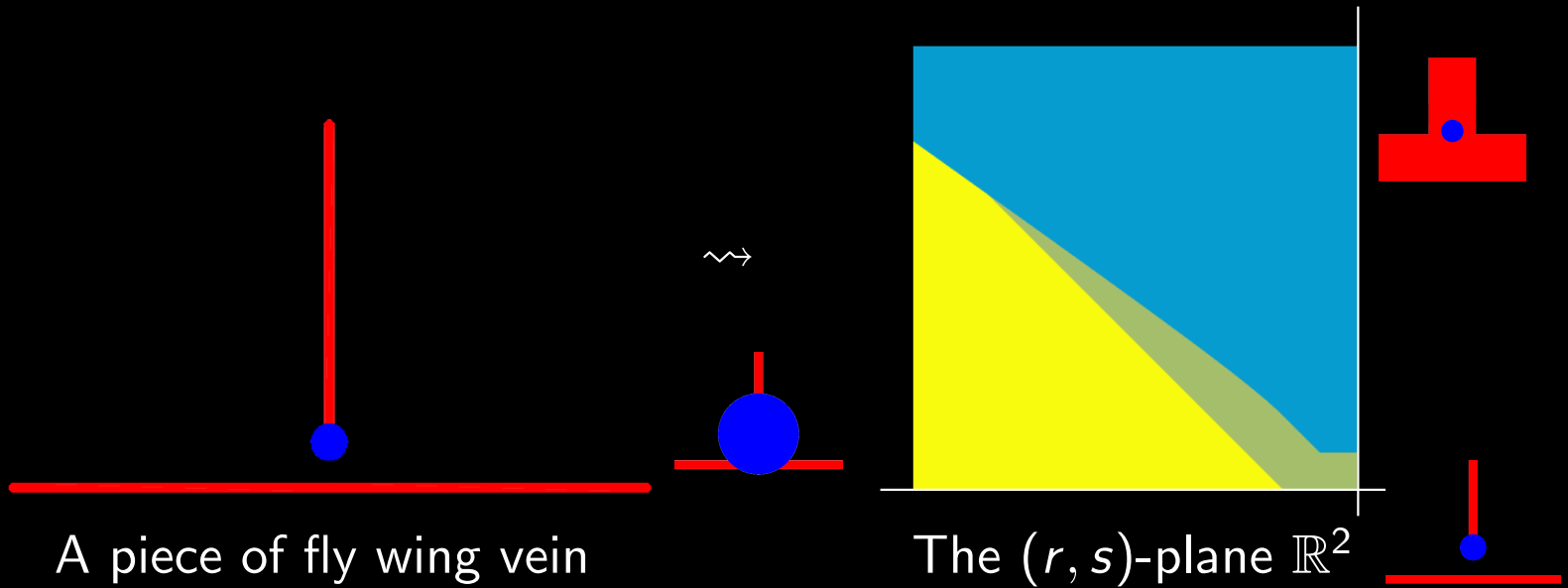

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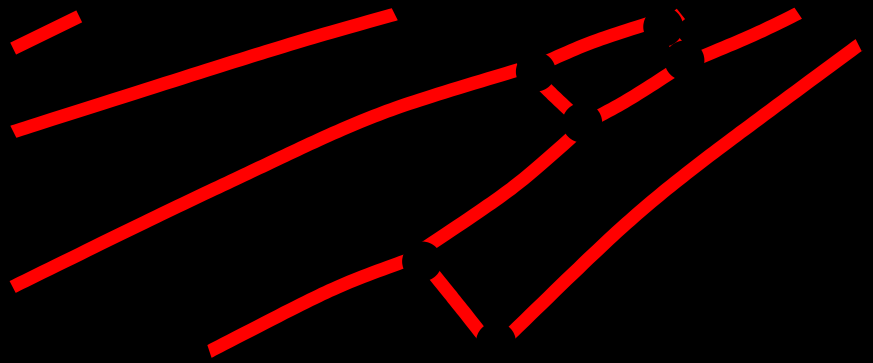

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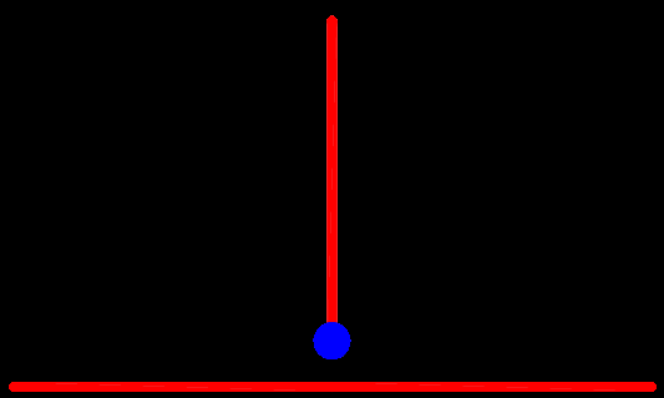

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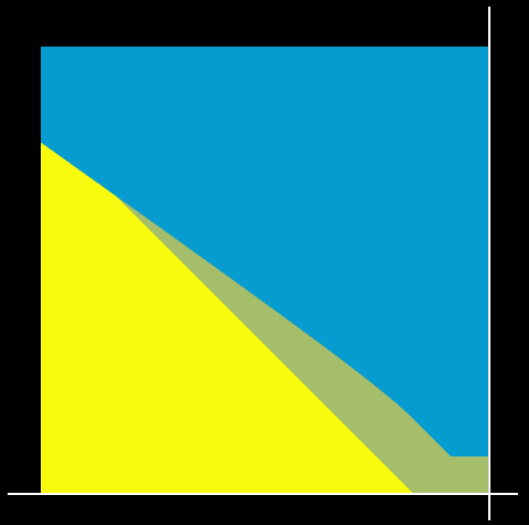

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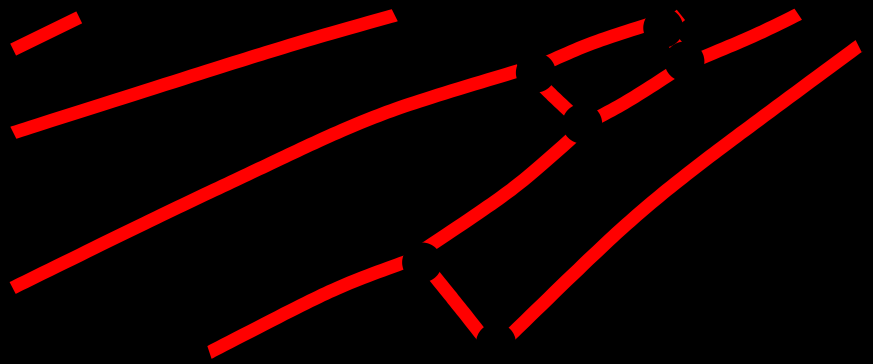

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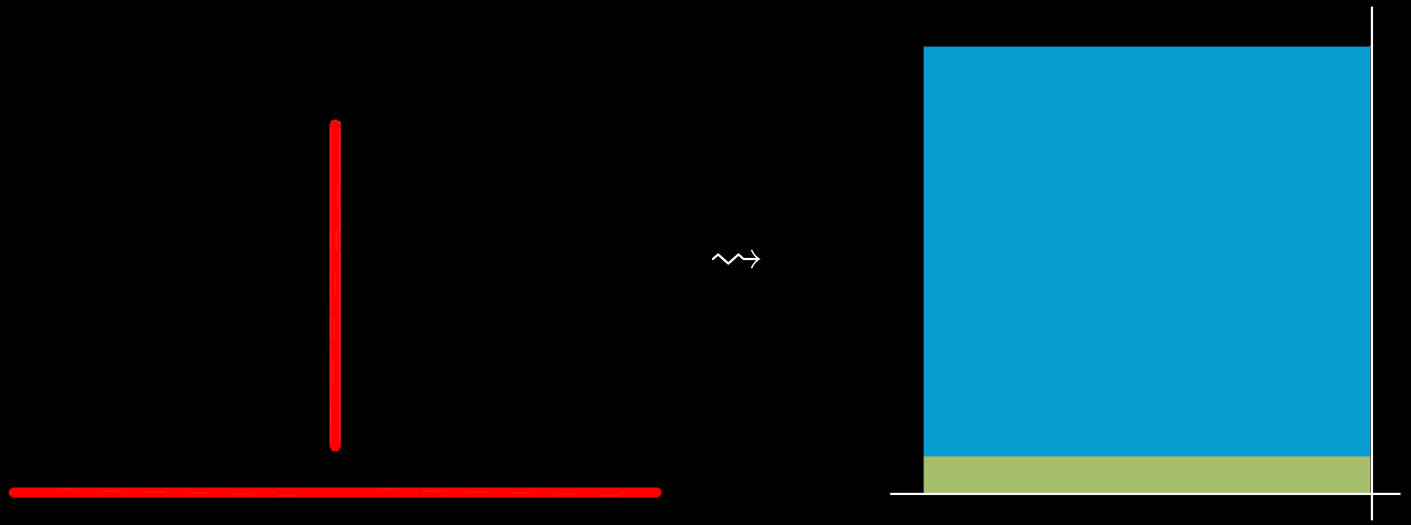

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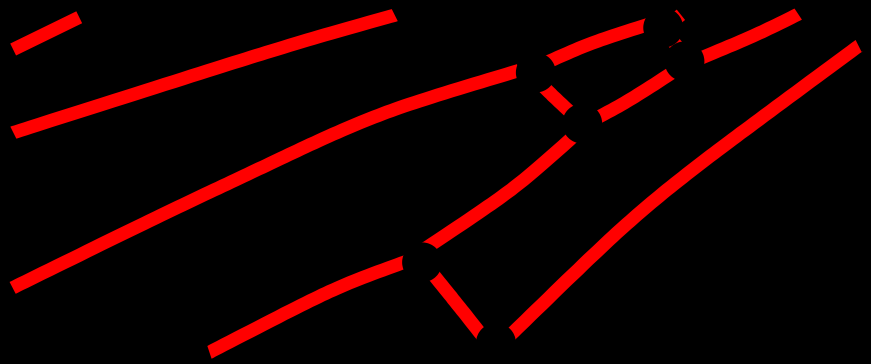

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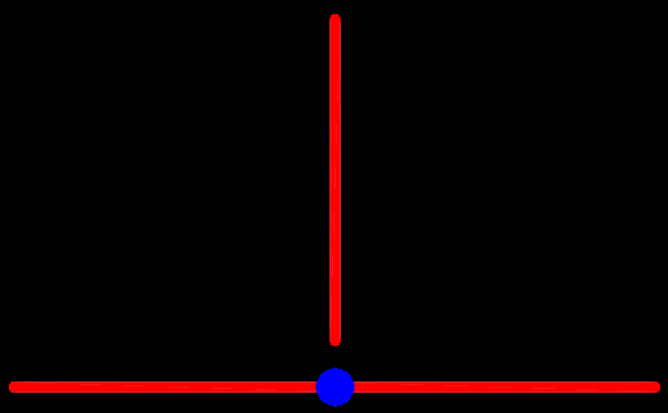

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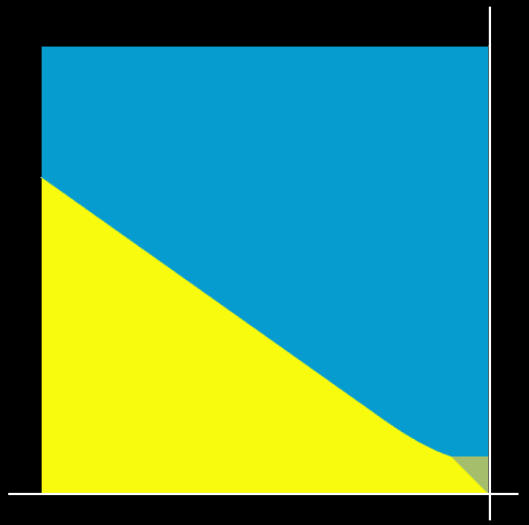

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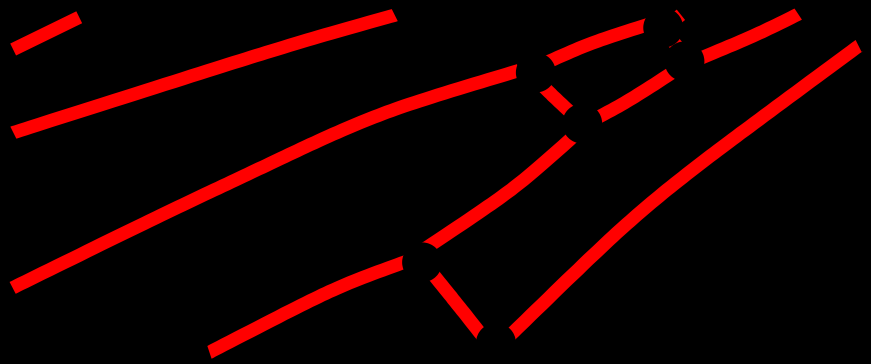

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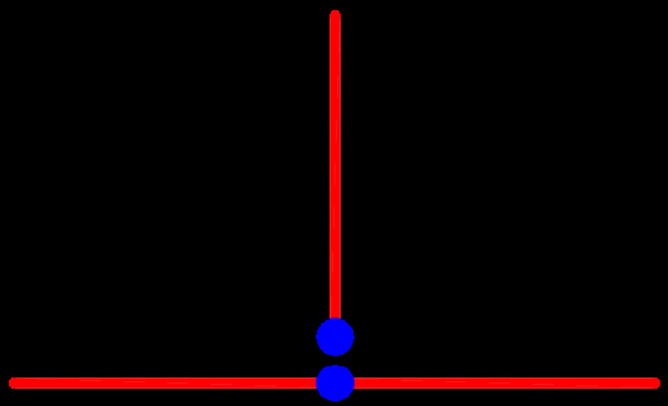

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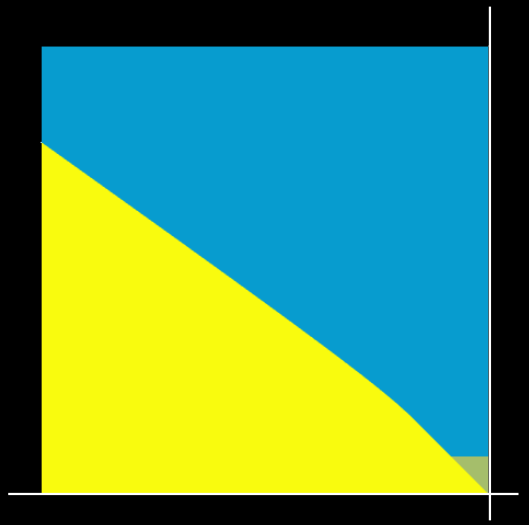

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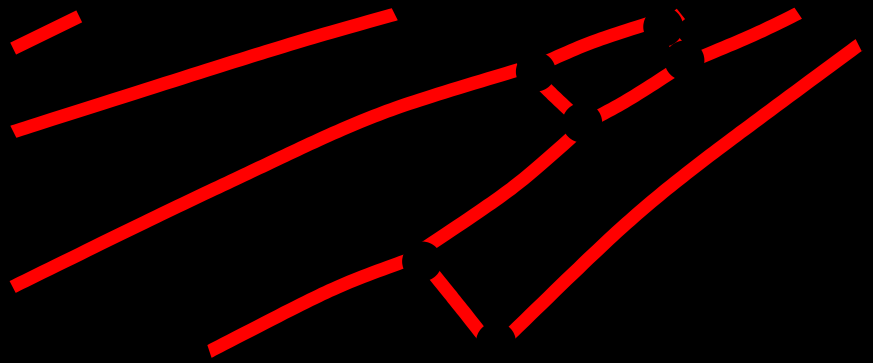

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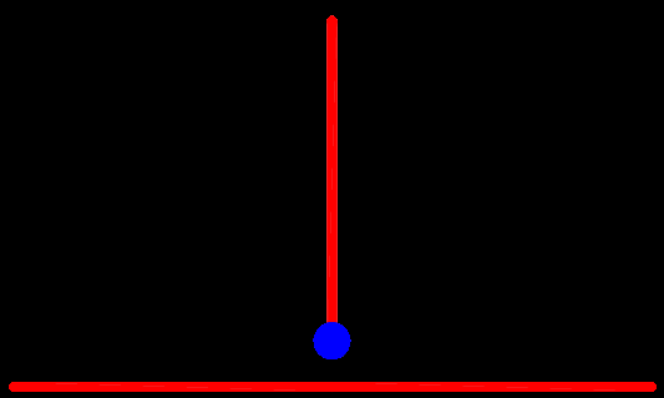

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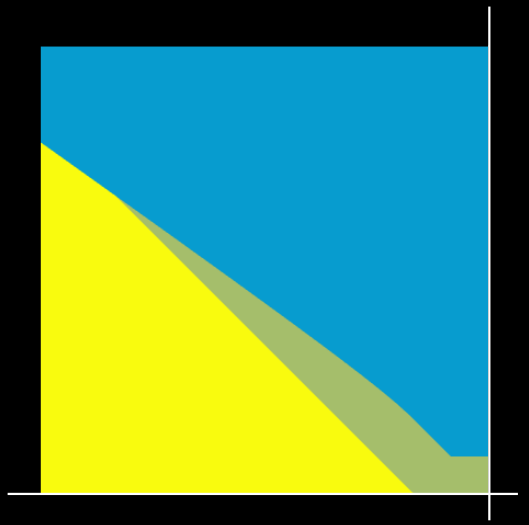

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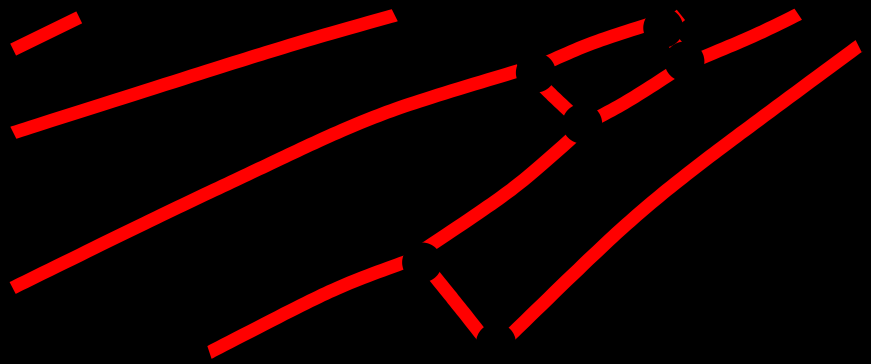

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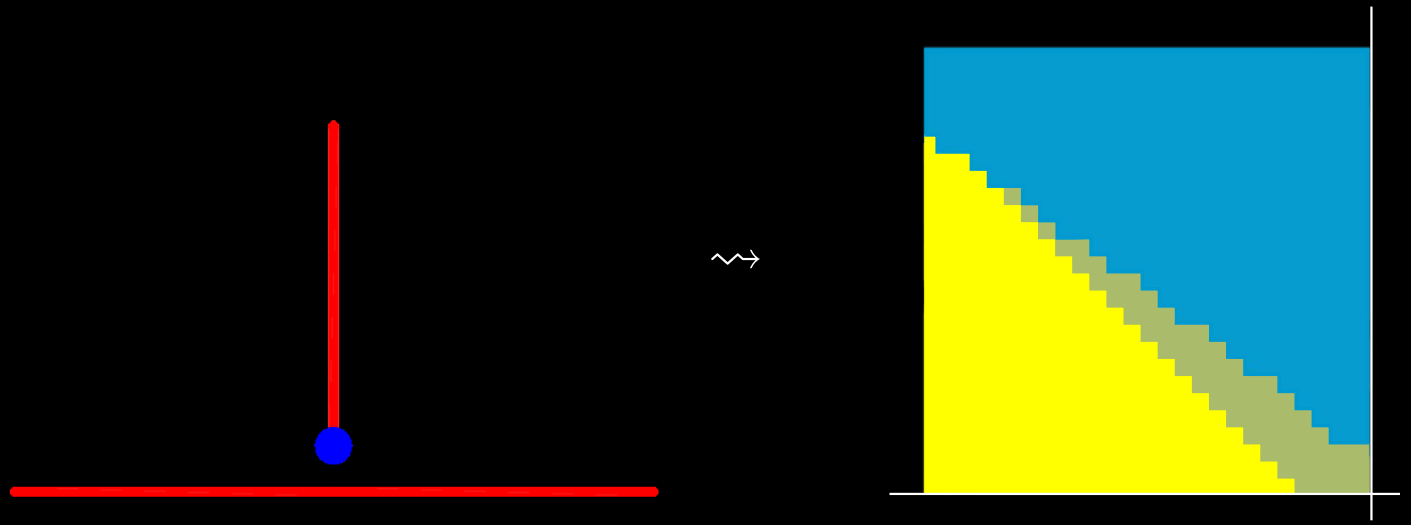

A piece of fly wing vein

discretized

Tameness

How to write down multipersistence modules in general? Need finiteness....

Def [M.– 2017, see arXiv:math.AT/2008.00063]. A module M over an arbitrary poset Q admits a constant subdivision if Q is partitioned into

- constant regions A, each with vector space $M_A \xrightarrow{\simeq} M_{\mathbf{a}}$ for all $\mathbf{a} \in A$, having
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M is tame if it admits a finite constant subdivision and $\dim_{\Bbbk} M_q < \infty$ for all q.

Example. $\Bbbk_{\mathbf{0}} \oplus \Bbbk[\mathbb{R}^2]$ admits constant regions $\{\mathbf{0}\}$ and $\mathbb{R}^2 \smallsetminus \{\mathbf{0}\}$

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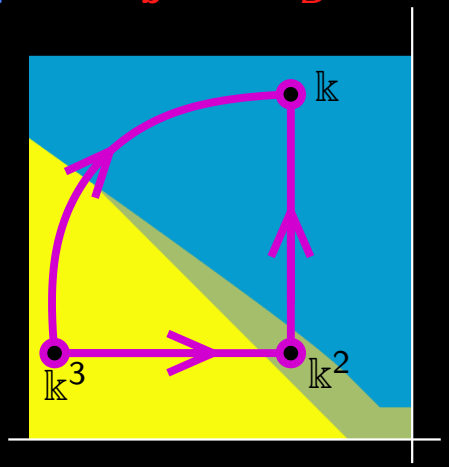

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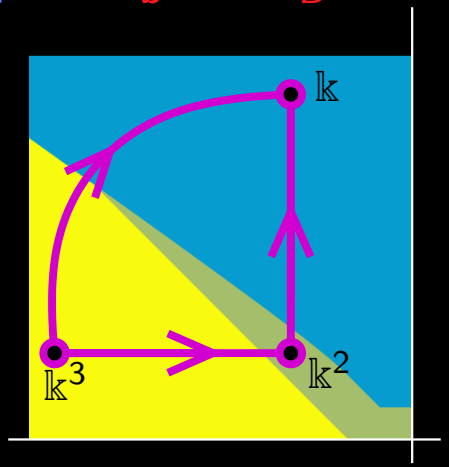

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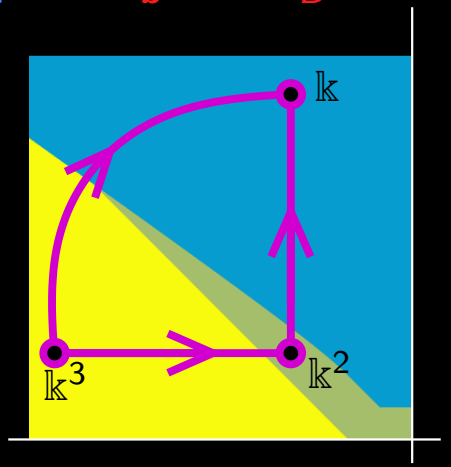

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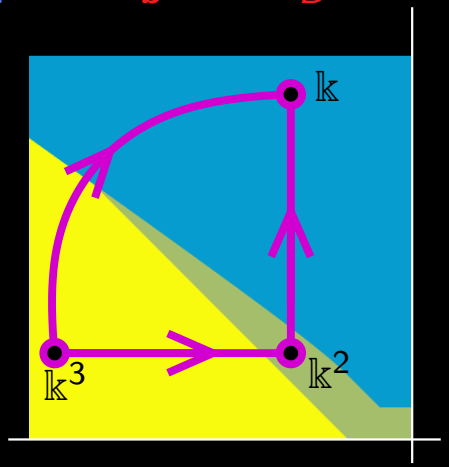
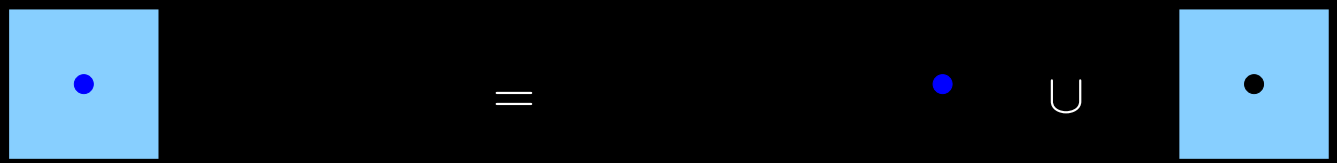
Def [M.– 2017, see arXiv:math.AT/2008.00063]. A module M over an arbitrary poset Q admits a constant subdivision if Q is partitioned into

- constant regions A, each with vector space $M_A \xrightarrow{\simeq} M_{\mathbf{a}}$ for all $\mathbf{a} \in A$, having
- no monodromy: all comparable pairs $\mathbf{a} \preceq \mathbf{b}$ with $\mathbf{a} \in A$ and $\mathbf{b} \in B$ induce the same composite $M_A \to M_{\mathbf{a}} \to M_{\mathbf{b}} \to M_B$.



M is tame if it admits a finite constant subdivision and $\dim_{\Bbbk} M_q < \infty$ for all q.

Example. $\Bbbk_{\mathbf{0}} \oplus \Bbbk[\mathbb{R}^2]$ admits constant regions $\{\mathbf{0}\}$ and $\mathbb{R}^2 \smallsetminus \{\mathbf{0}\}$



Encoding persistence modules

Def. A module M over a poset Q has finite encoding $\pi : Q \to P$ if

- P is a finite poset,
- π is a poset morphism, and
- $M \cong \pi^* N = \bigoplus_{q \in Q} N_{\pi(q)}$, the pullback of P-module N.

Thm [M.– 2017, see arXiv:math.AT/2008.00063]. tame $\Leftrightarrow$ finitely encodable

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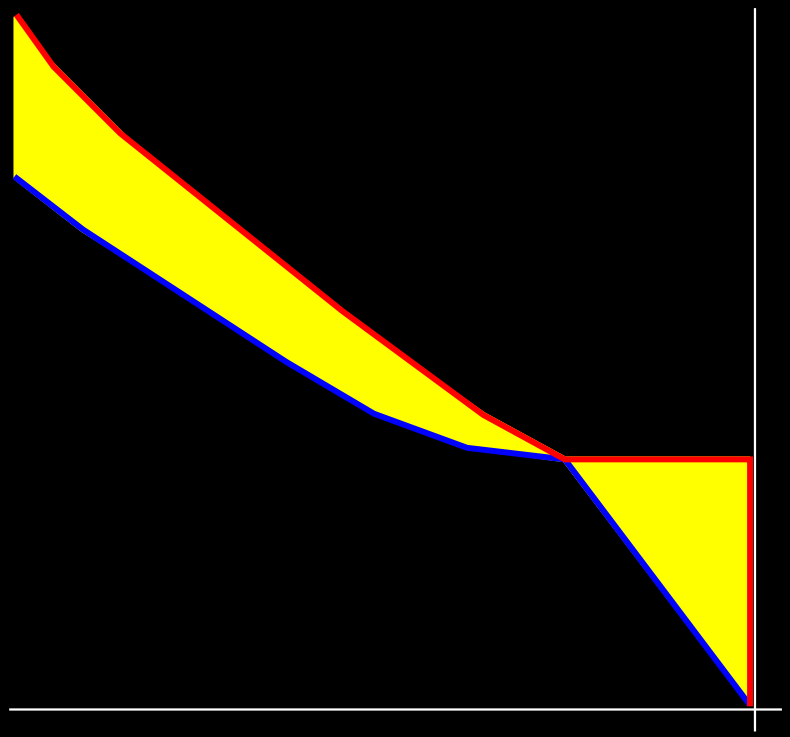

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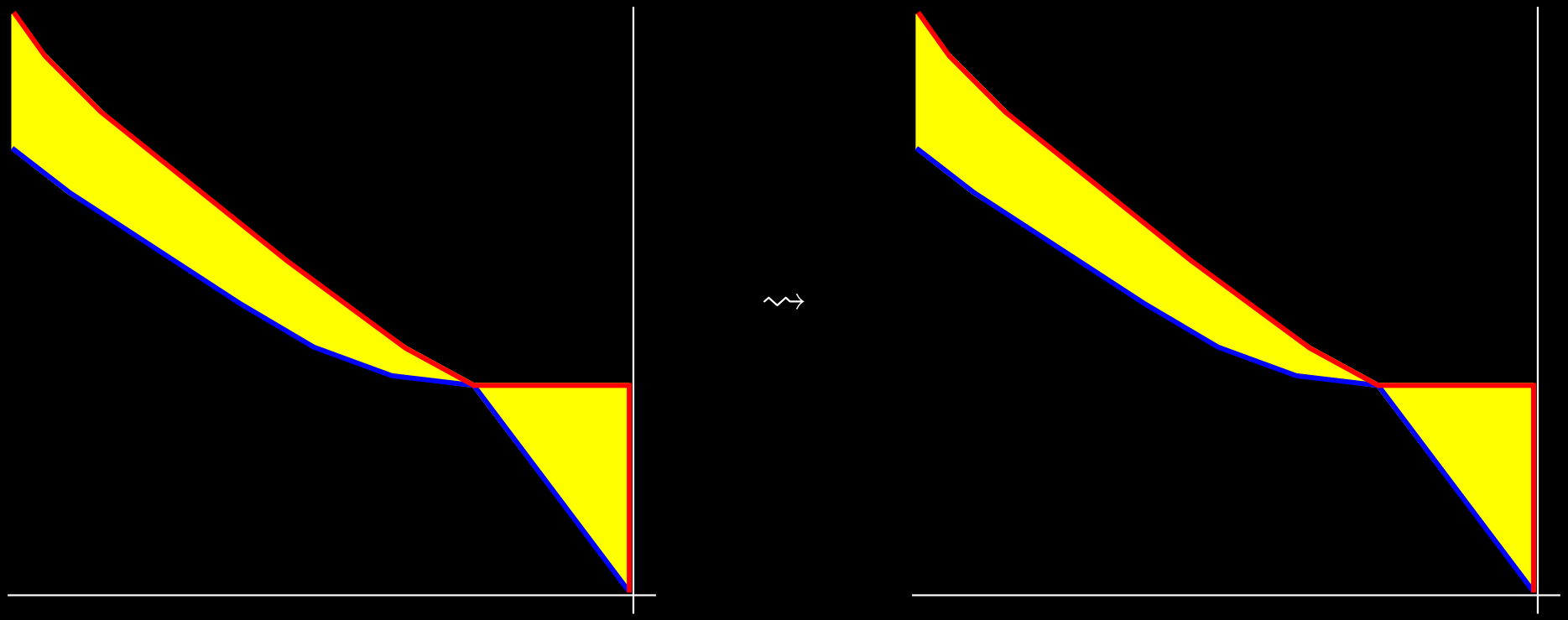

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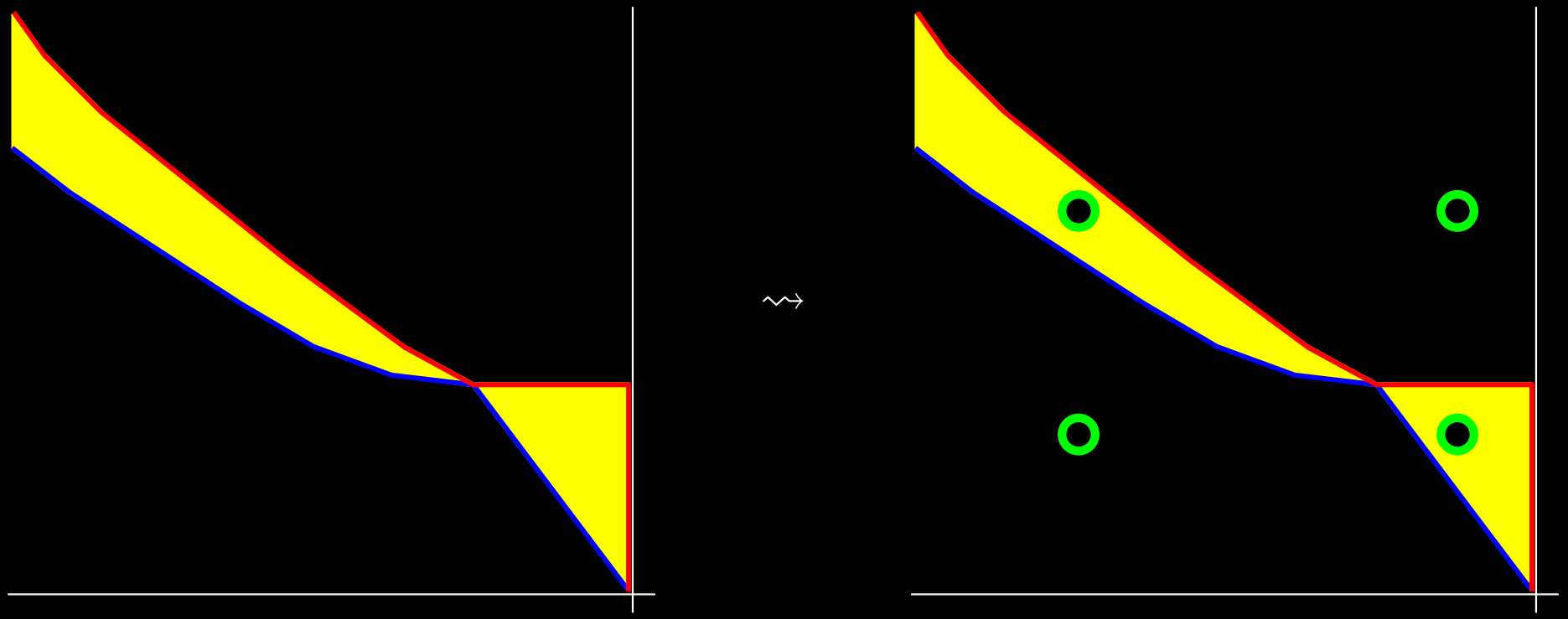

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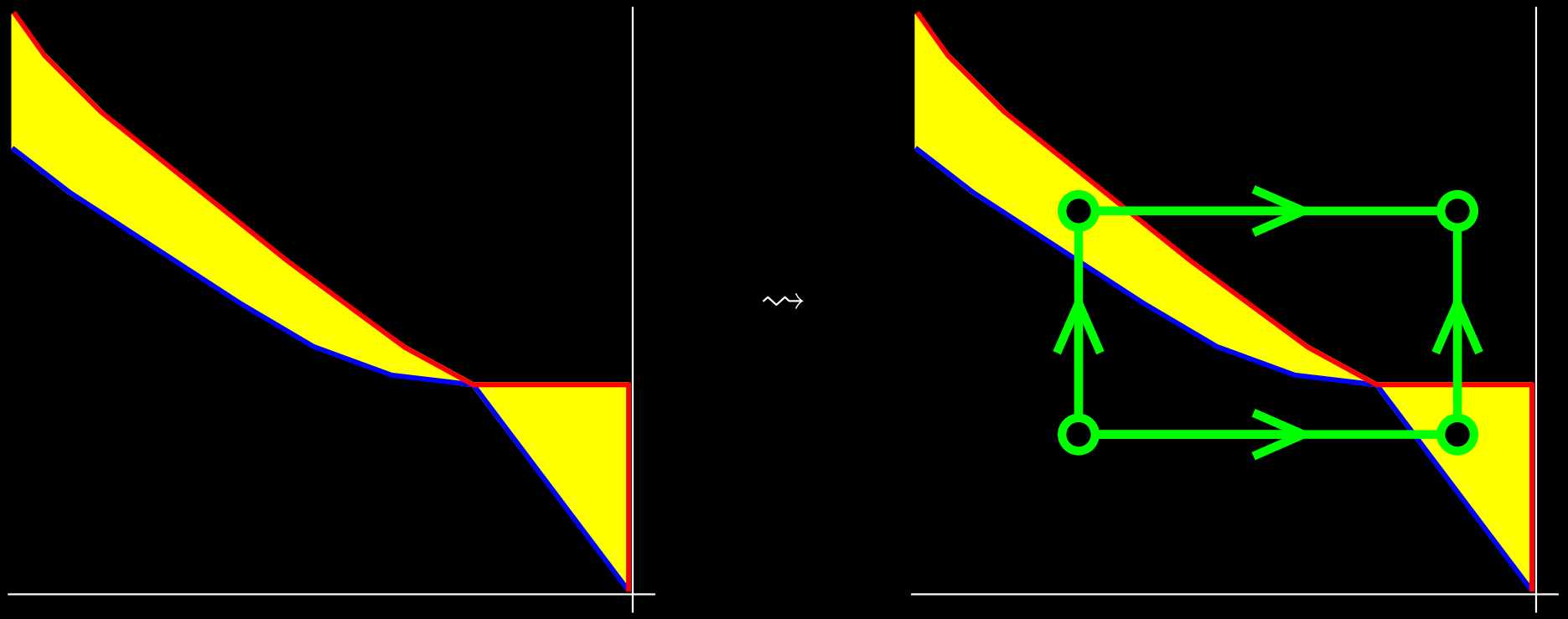

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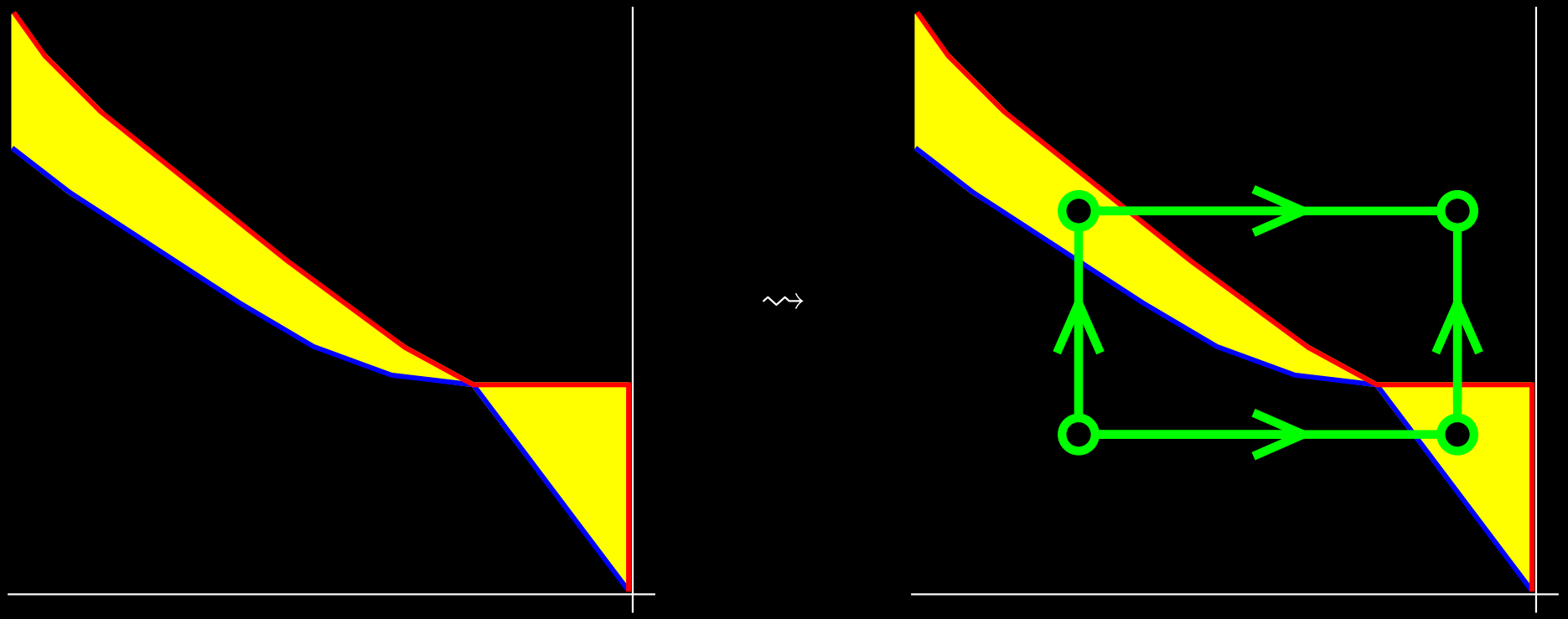

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Input. Topological space X filtered by set Q of subspaces: $X_q \subseteq X$ for $q \in Q$
$\Rightarrow$ Q is a partially ordered set: $X_q \subseteq X_{q'} \Leftrightarrow q \preceq q'$

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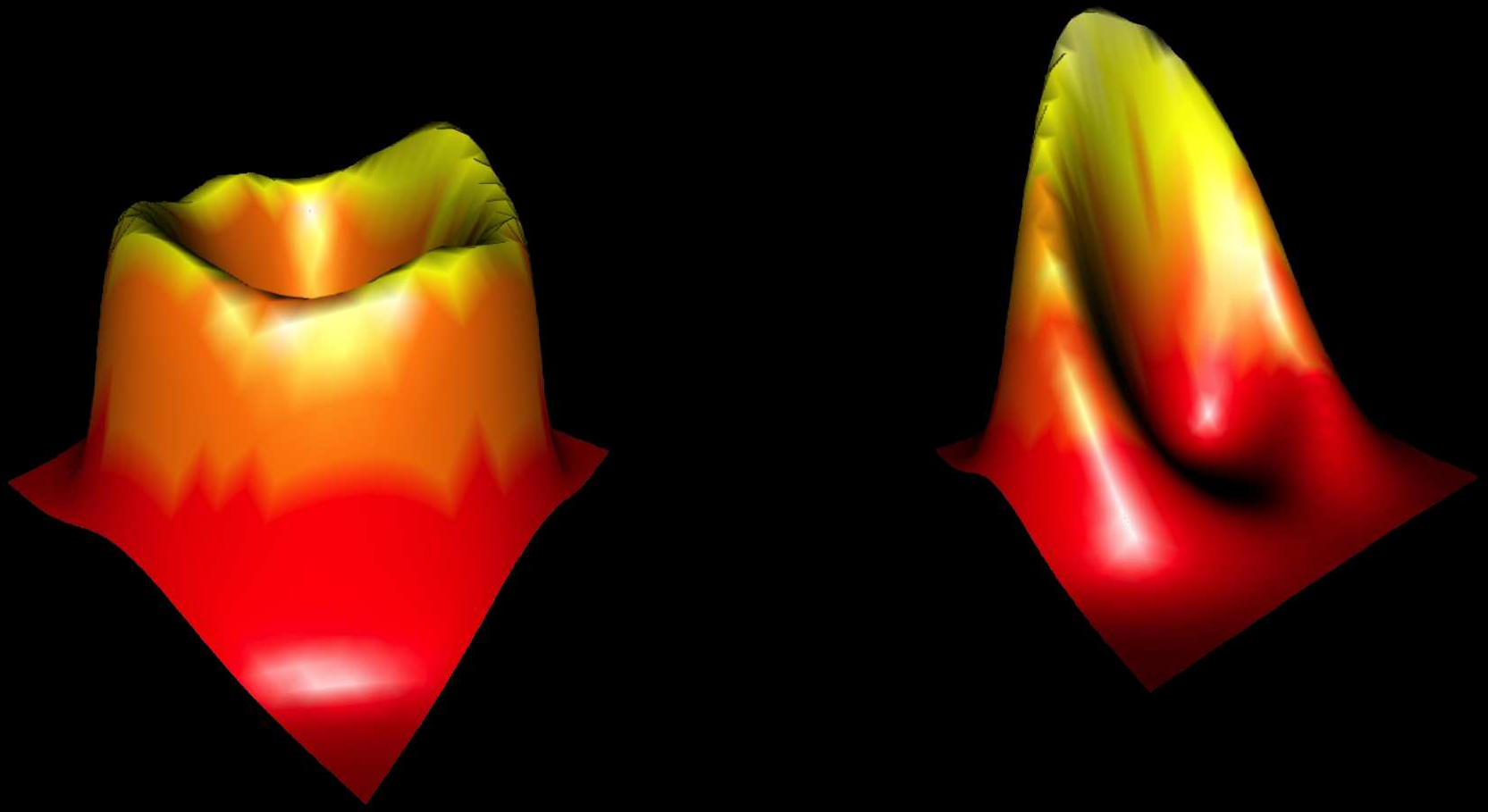
Topology of probability distributions



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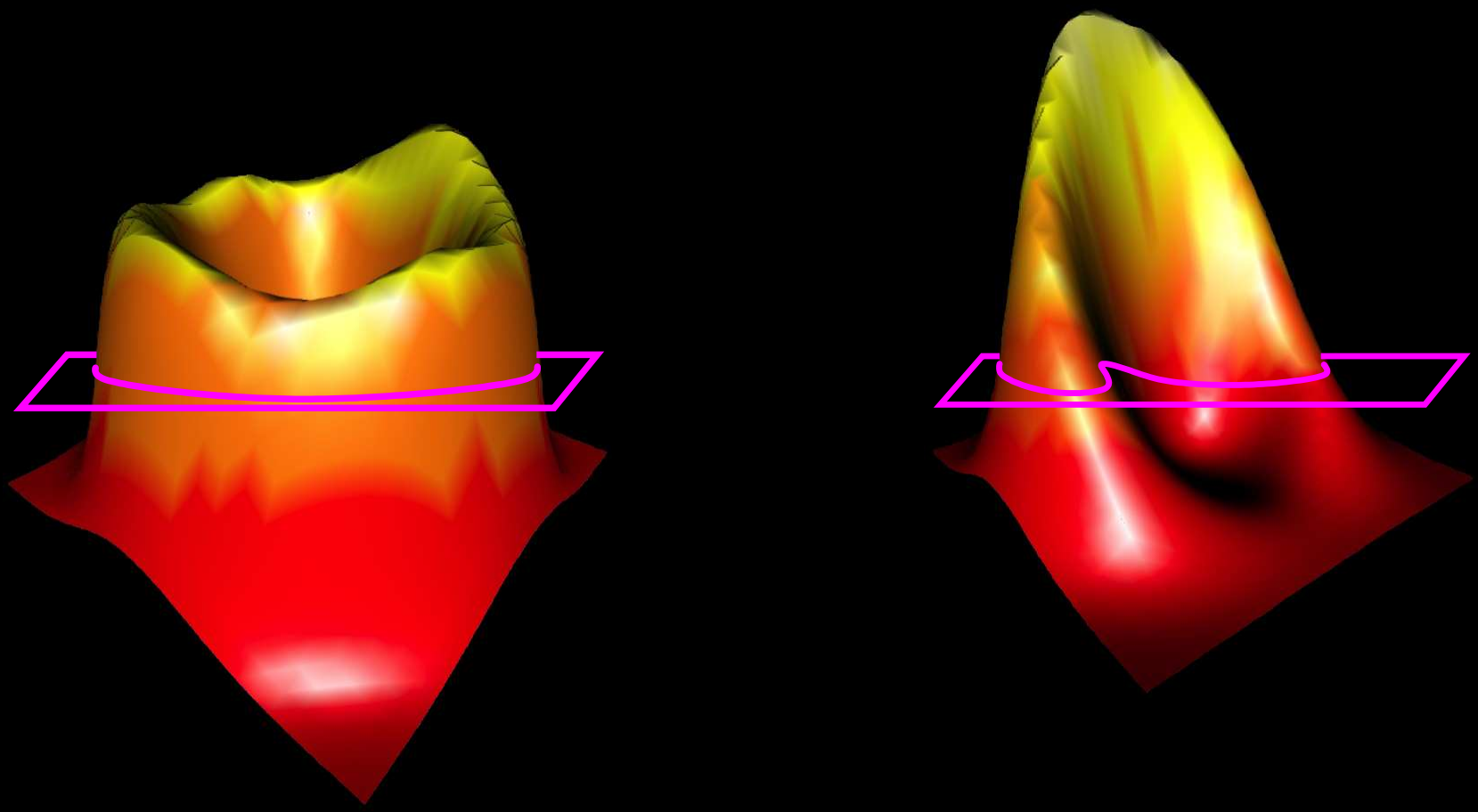

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History of persistent homology

Ordinary persistence

- traces back to [Morse 1940s]
- bar codes [Abeasis–Del Fra 1980], rediscovered many times
- formally defined [Frosini, Landi 1999], [Robins 1999]
- efficient computation [Edelsbrunner, Letscher, Zomorodian 2002]
- applications [too many to list; a few early ones, but most roughly 2013–]

Multiparameter persistence

- introduced [Carlsson, Zomorodian 2009]
- algorithms, presentations, visualizations, notions of noise, distance, . . .
  [Bubenik, Carlsson, Chachólski, Lesnick, Scolamiero, Vaccarino, Wright, Zomorodian,. . .]
  + usually assume finitely presented, even if over $\mathbb{R}^n$

Essentially equivalent

- representation of Q [Nazarova–Roiter 1972]
- functor from Q to the category of vector spaces (e.g., [Curry 2019])
- vector-space valued sheaf on Q (e.g., [Yuzvinsky 1987], [Yanagawa 2001], [Curry 2014])
- representation of incidence algebra of Q [Doubilet–Rota–Stanley 1972]
- module over directed acyclic graph Q [Chambers–Letscher 2018]
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Brain artery analysis

Goal: statistical analysis, correlate with age or sex, taking into account

- 3D structure, in particular
- "bendiness", or "tortuosity"

Discrete methods [Aydin, et al. 2009]

- disregard metric and embedding
- compare combinatorial structures
- no correlations detected

Phylogenetic trees [SAMSI WG 2013]

- connect cortical surface landmarks to nearest leaves
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Method

Sweep filtration

Filter brain arteries by sweeping across with a plane:

Record:

- birth time of each new component
- death of each component (when it joins to an older component)

Easily computable (if $\dim X$ is low; ambient space dim irrelevant).

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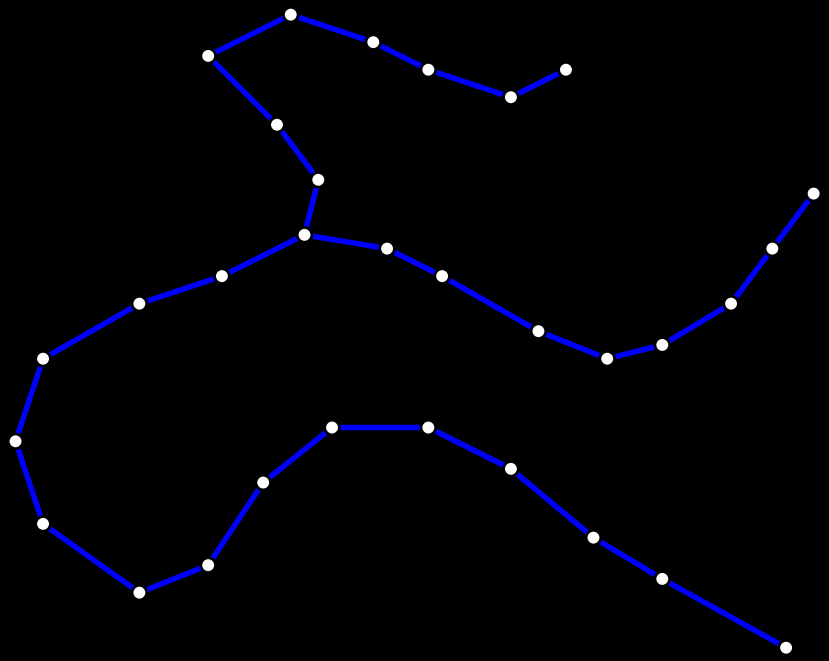

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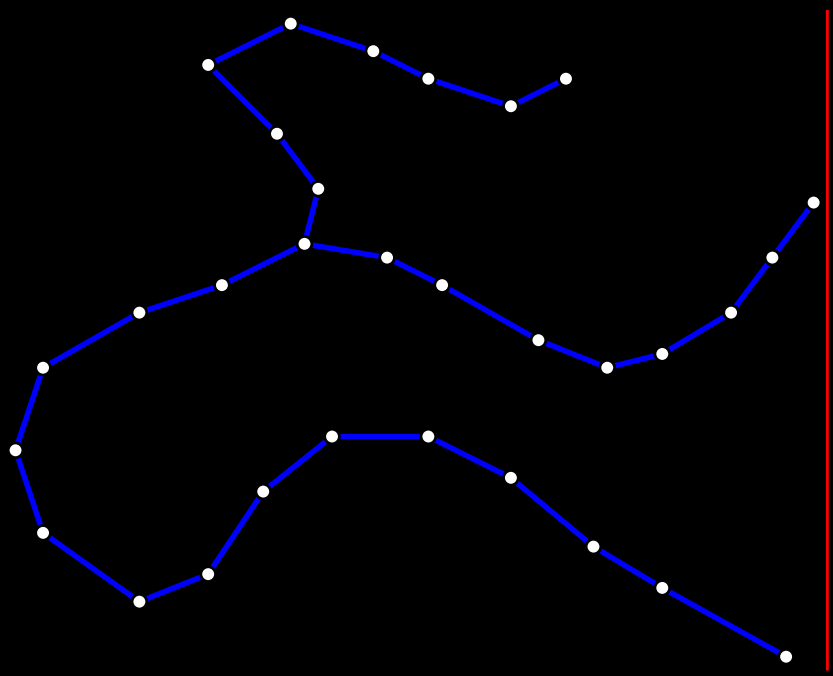

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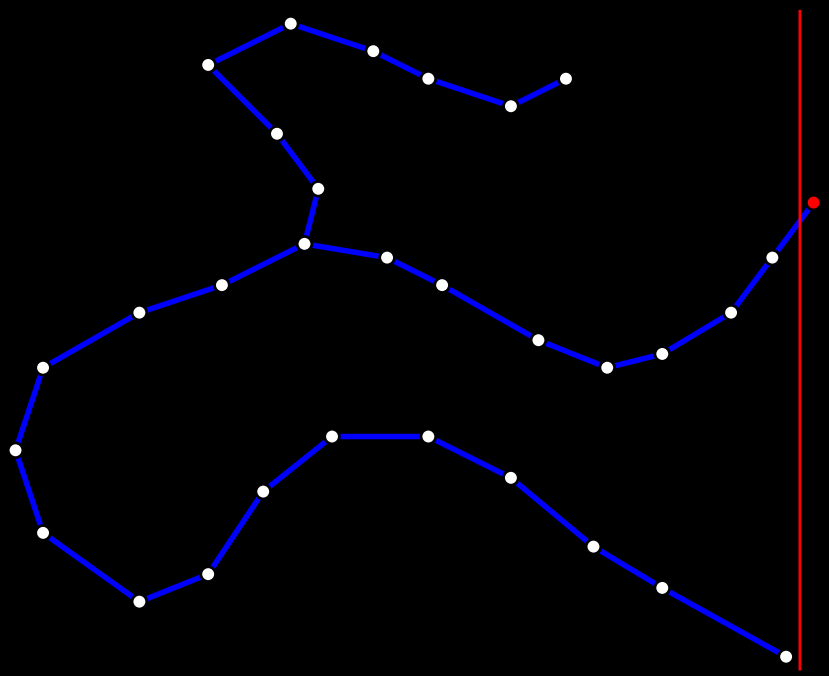

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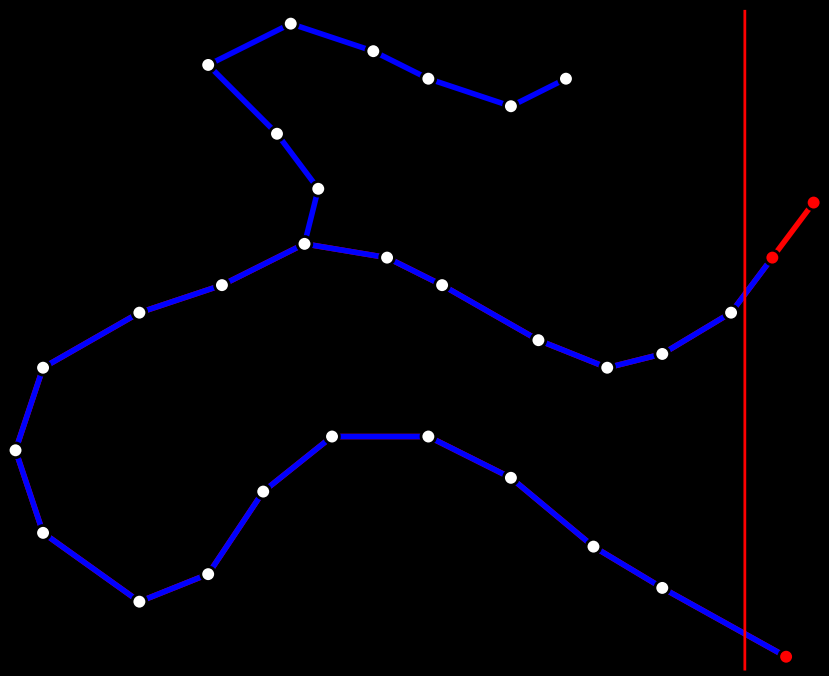

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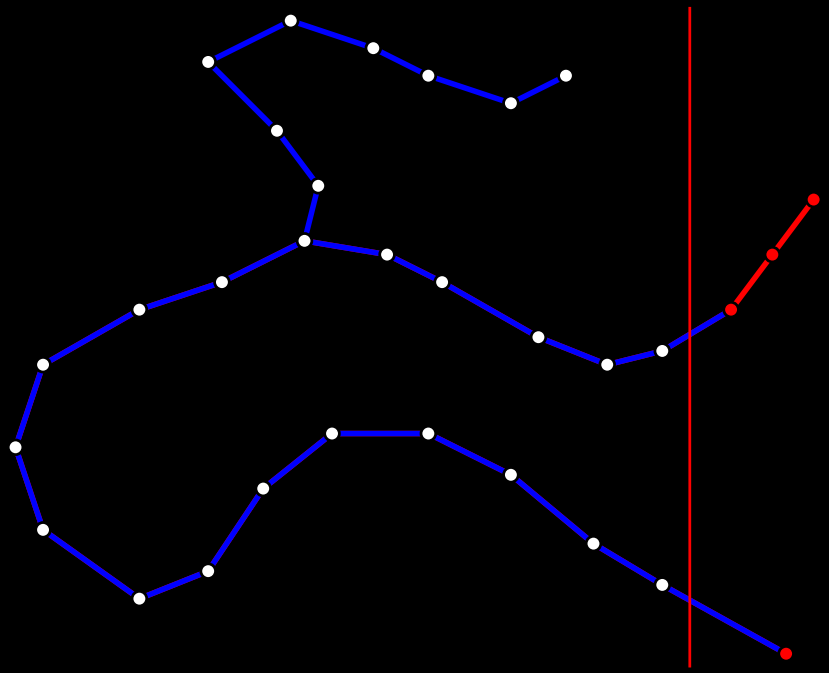

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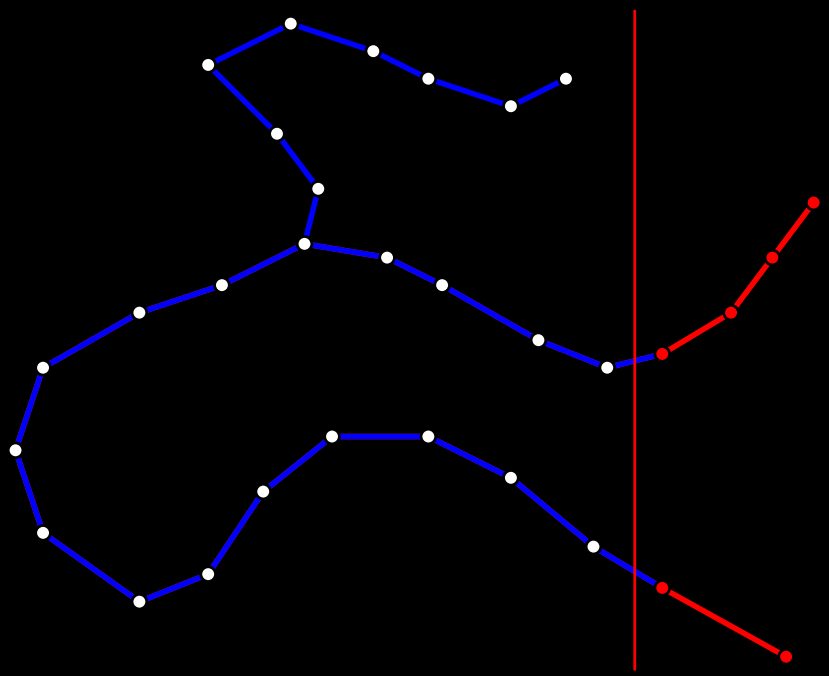

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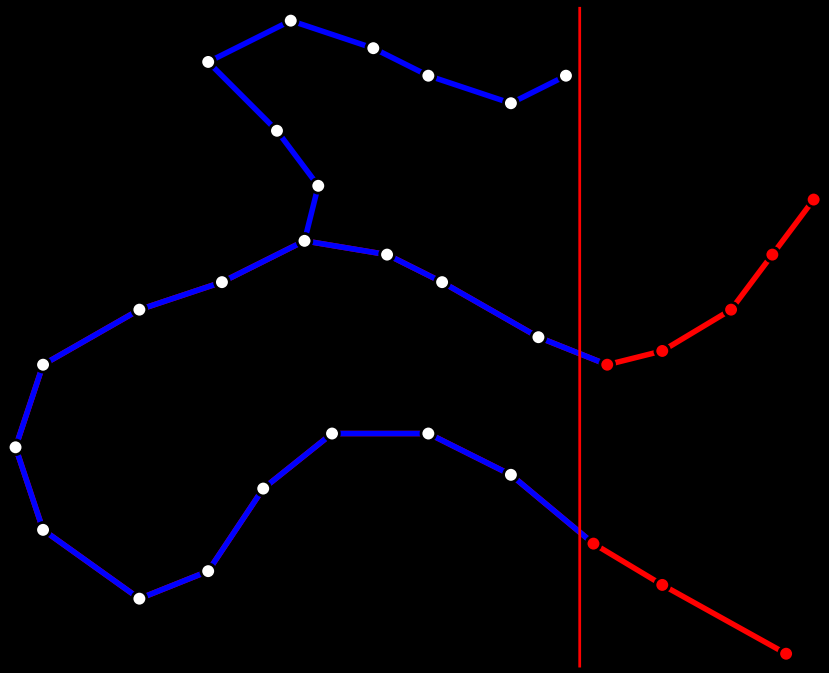

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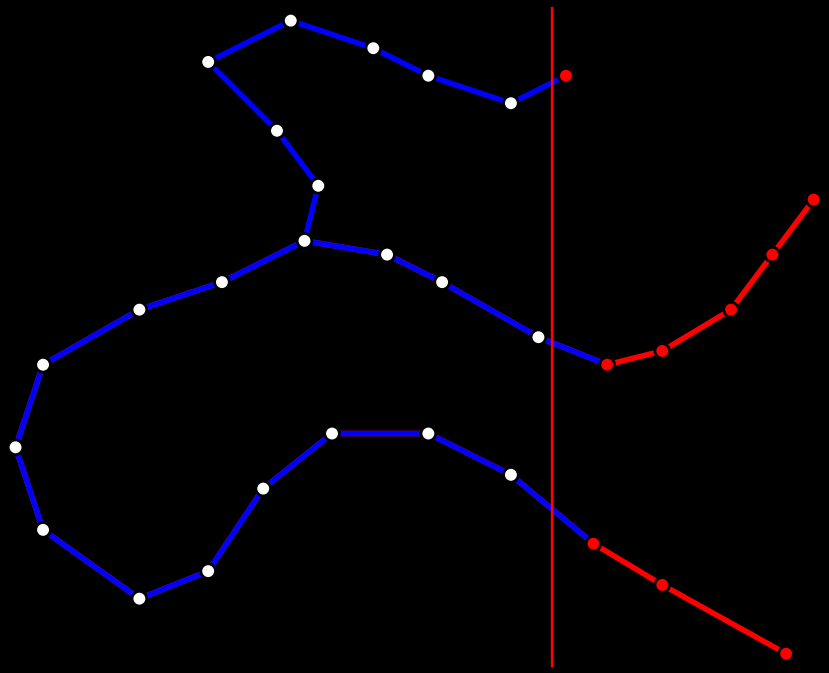

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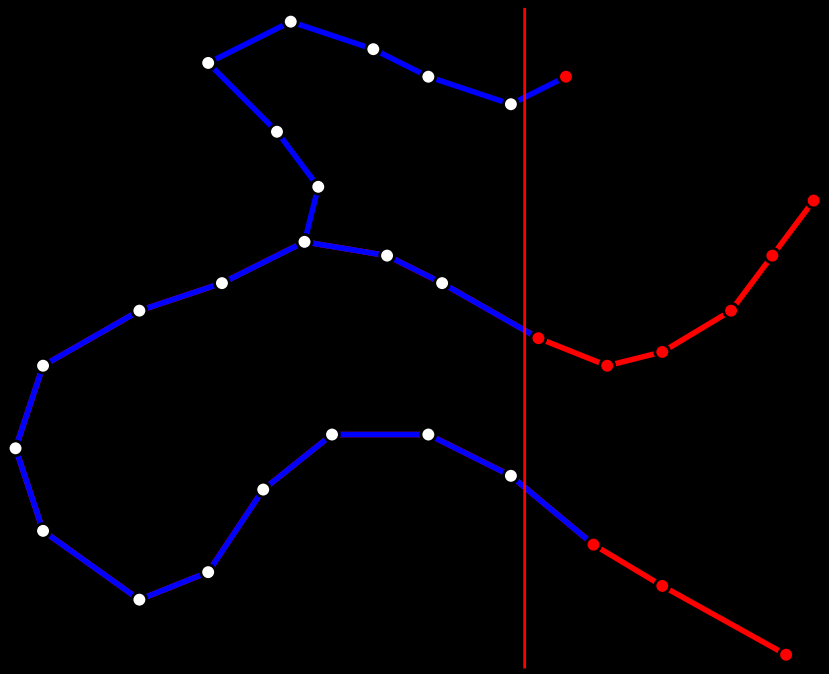

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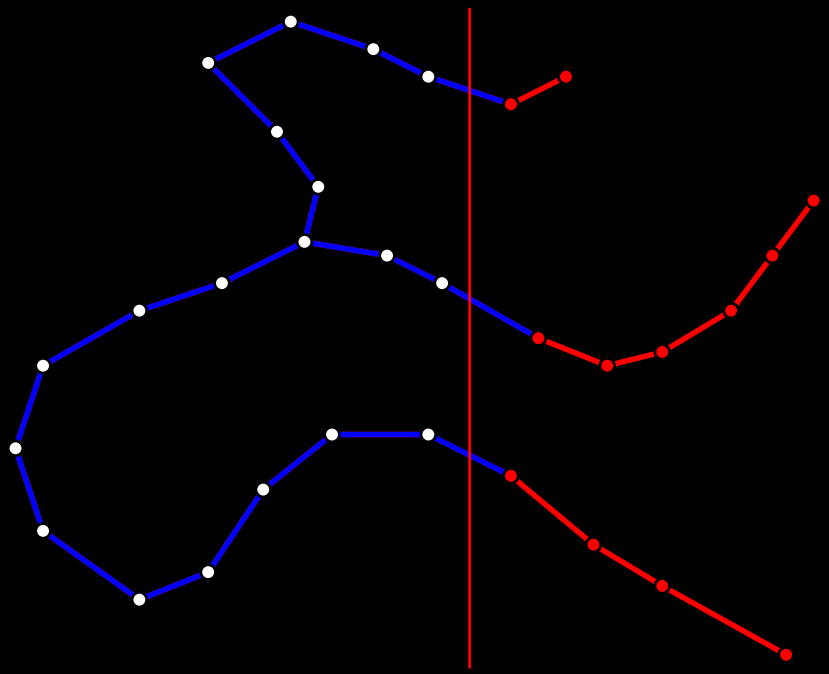

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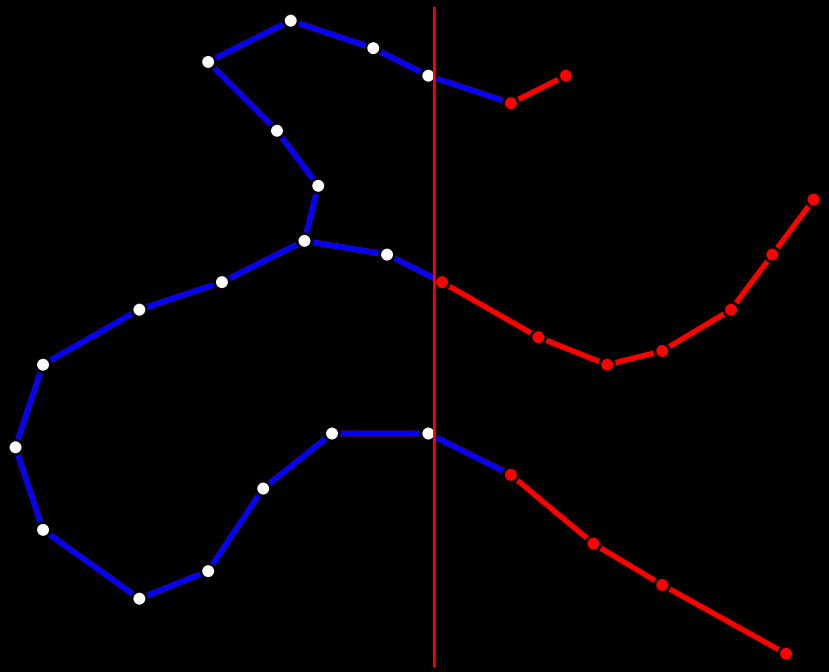

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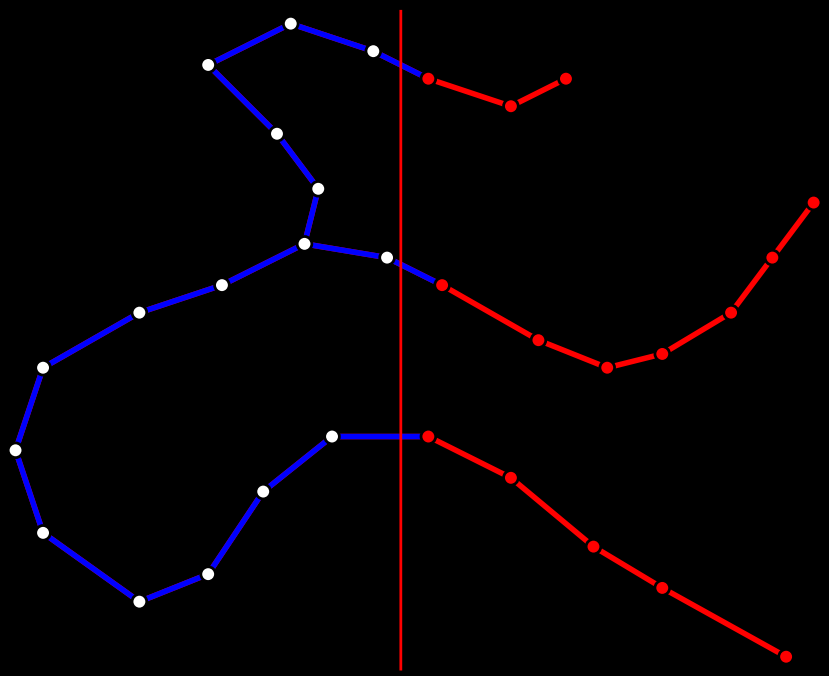

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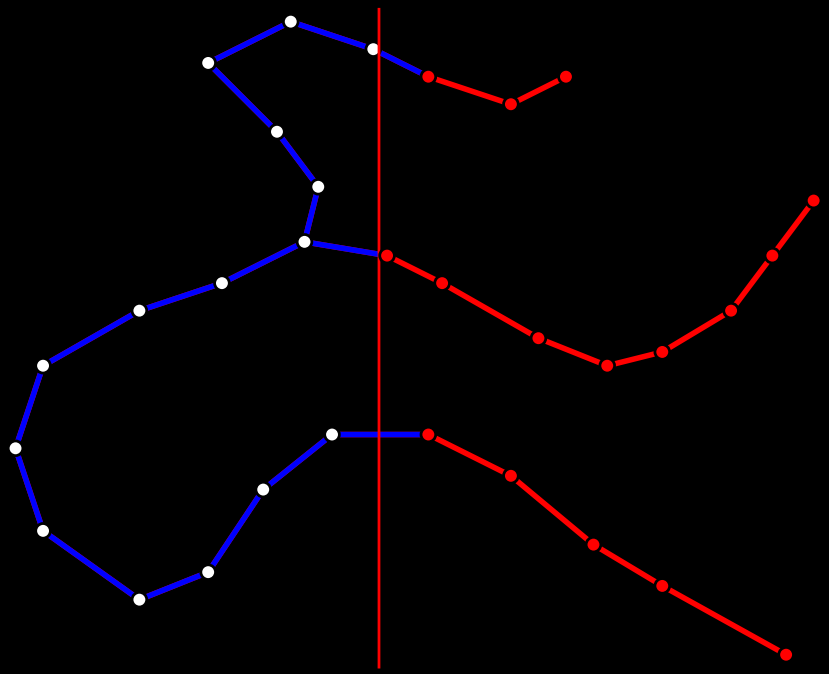

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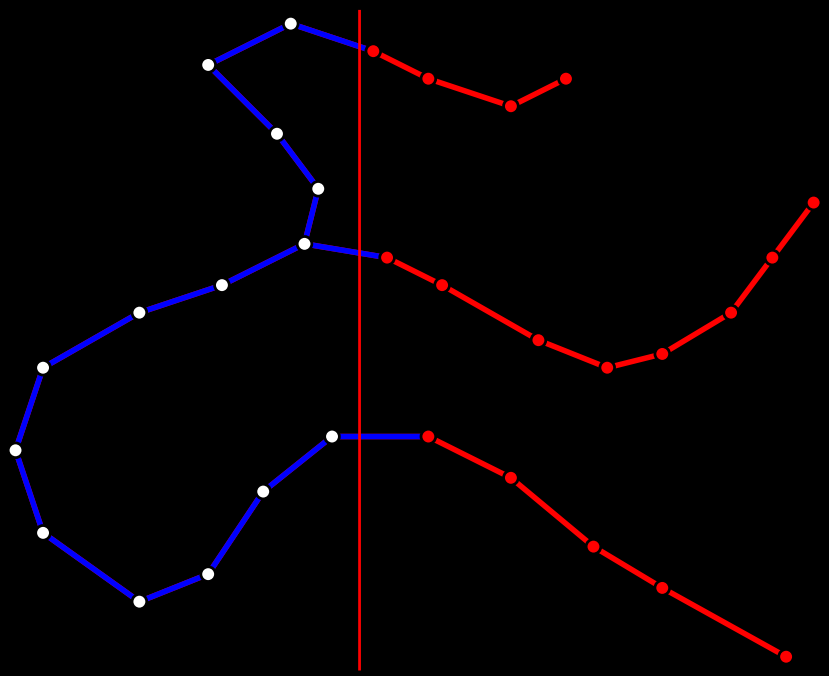

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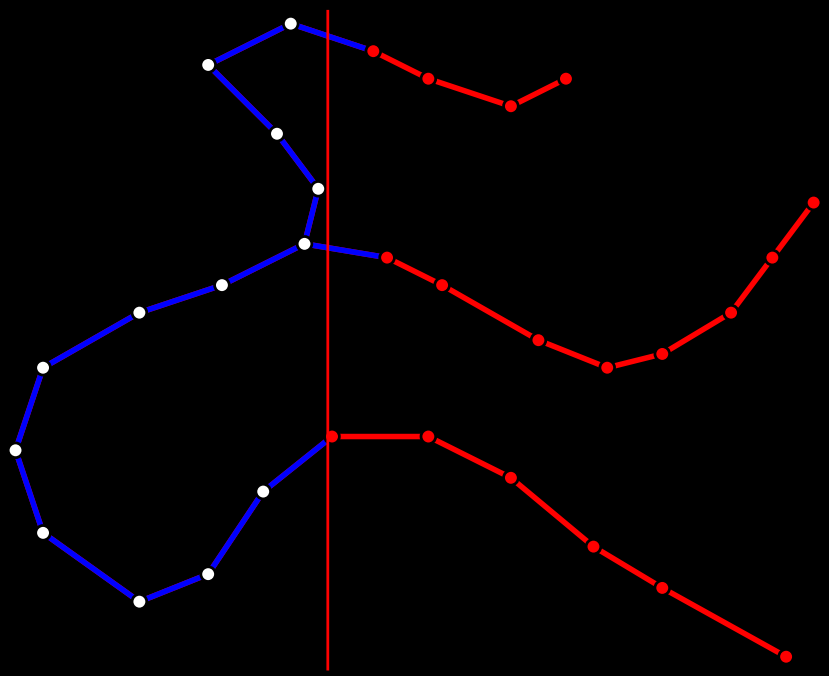

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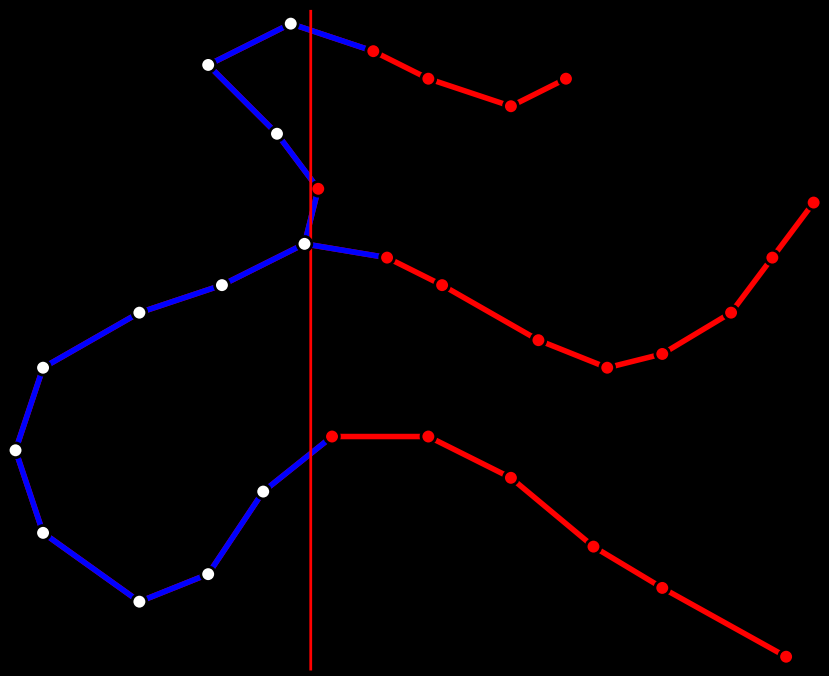

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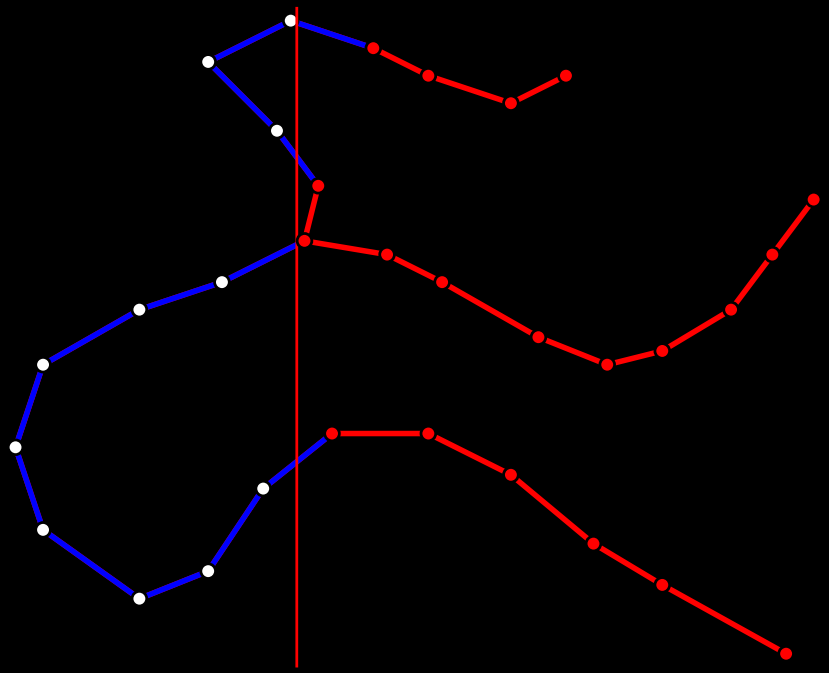

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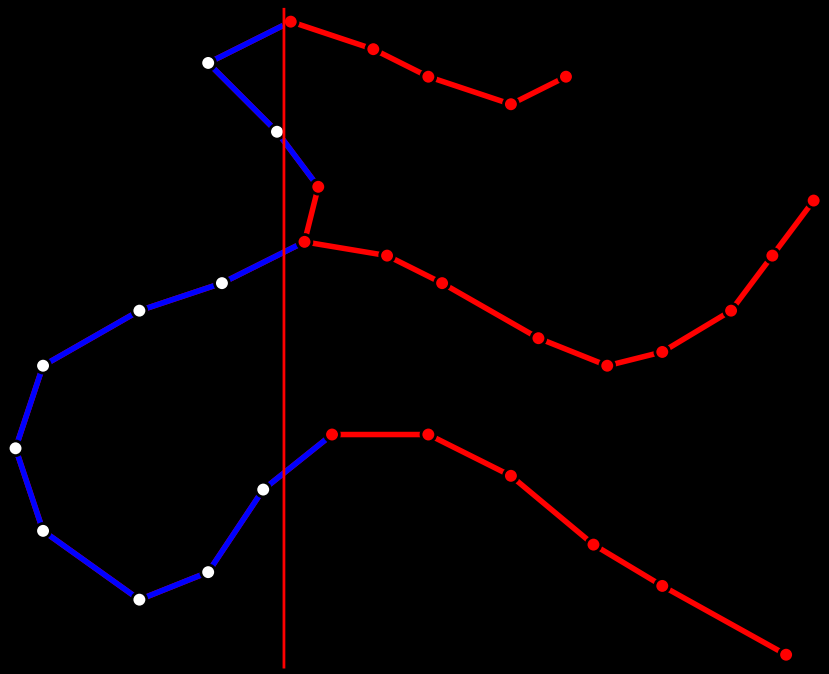

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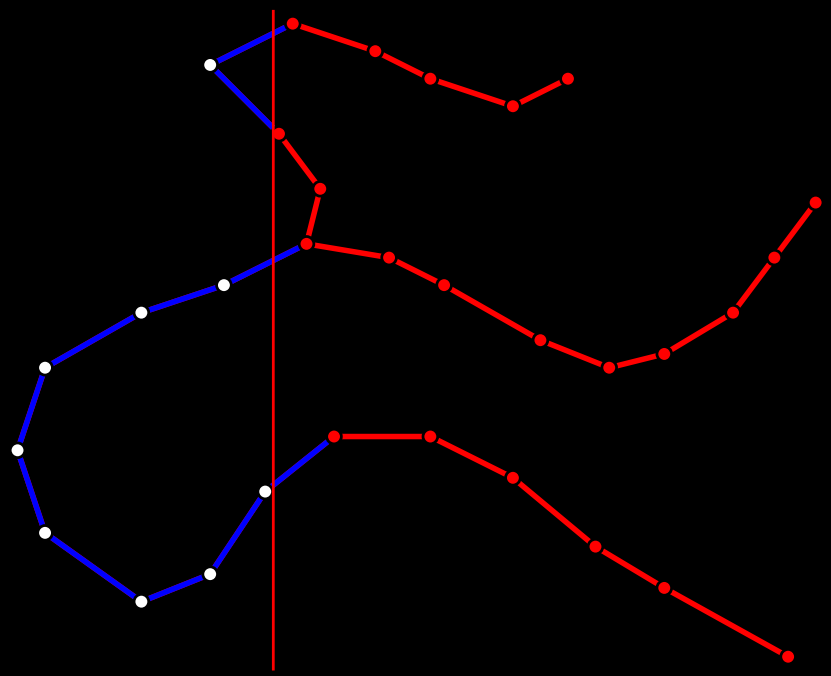

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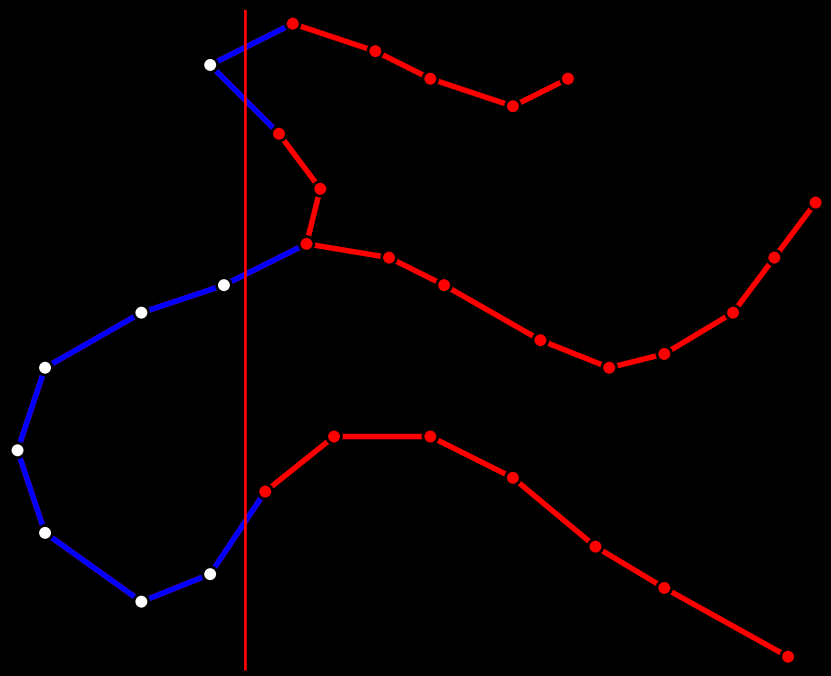

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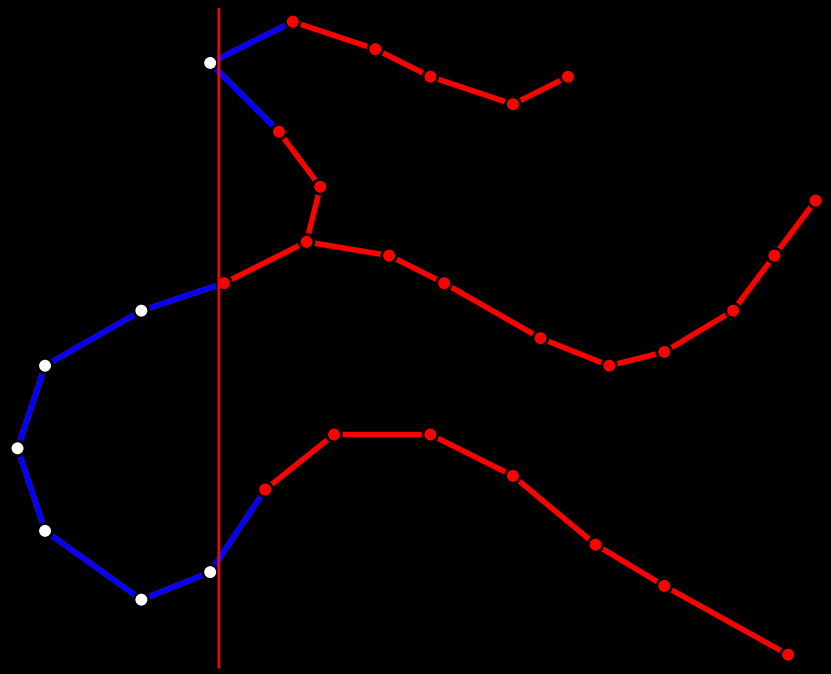

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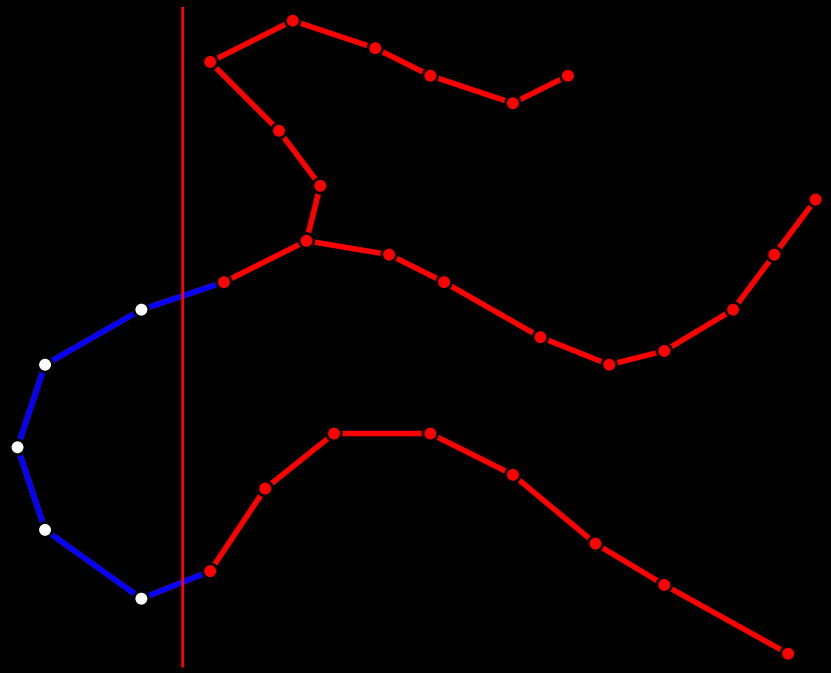

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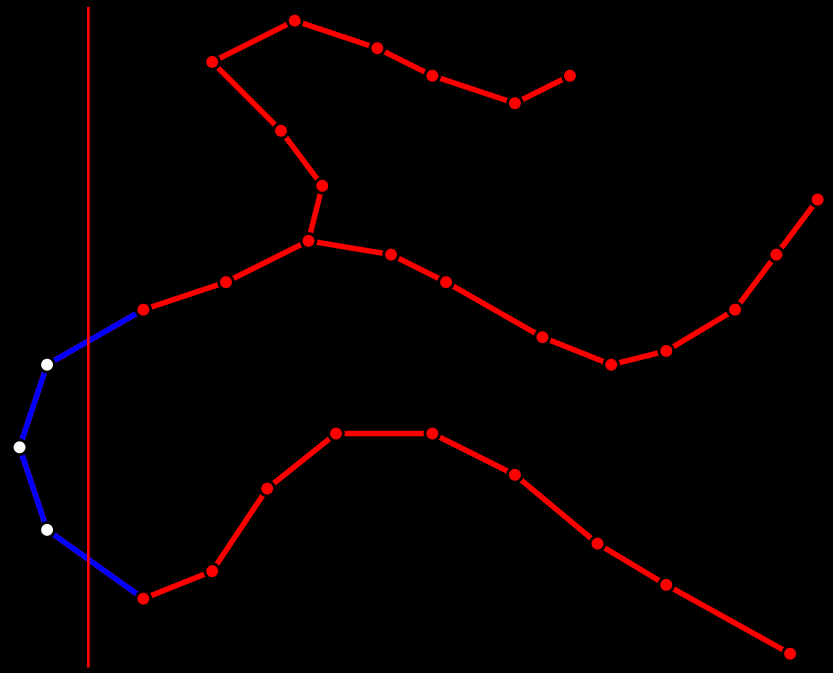

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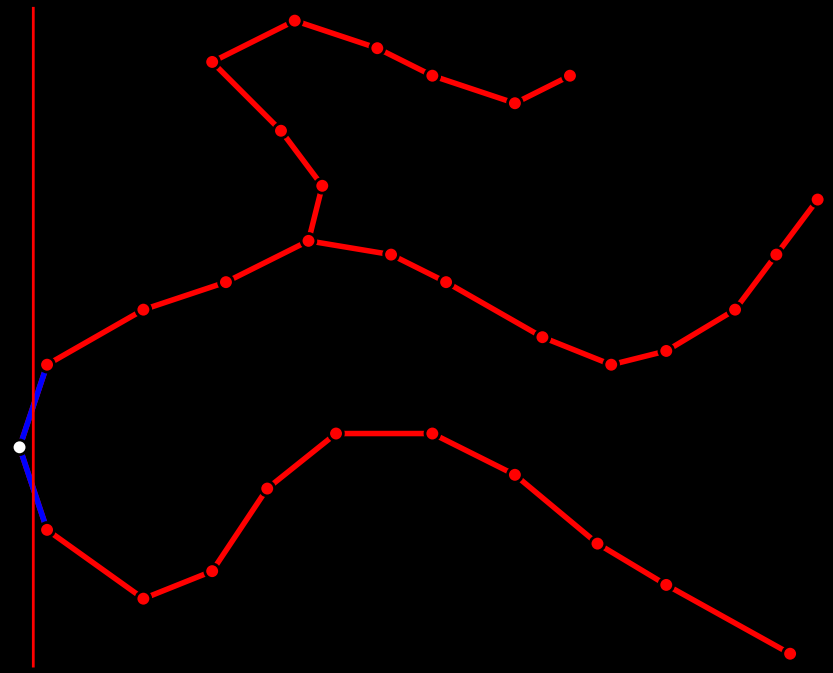

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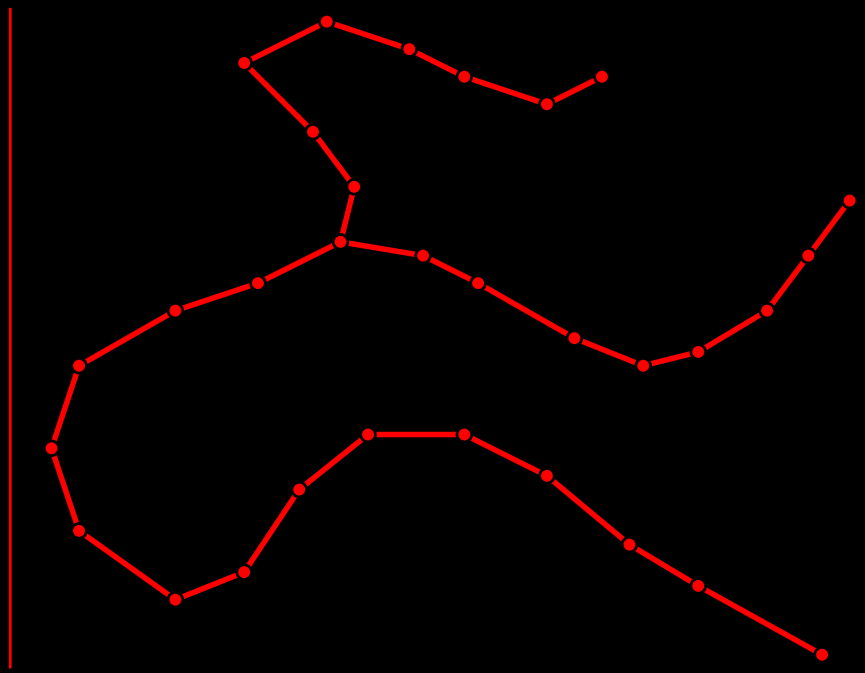

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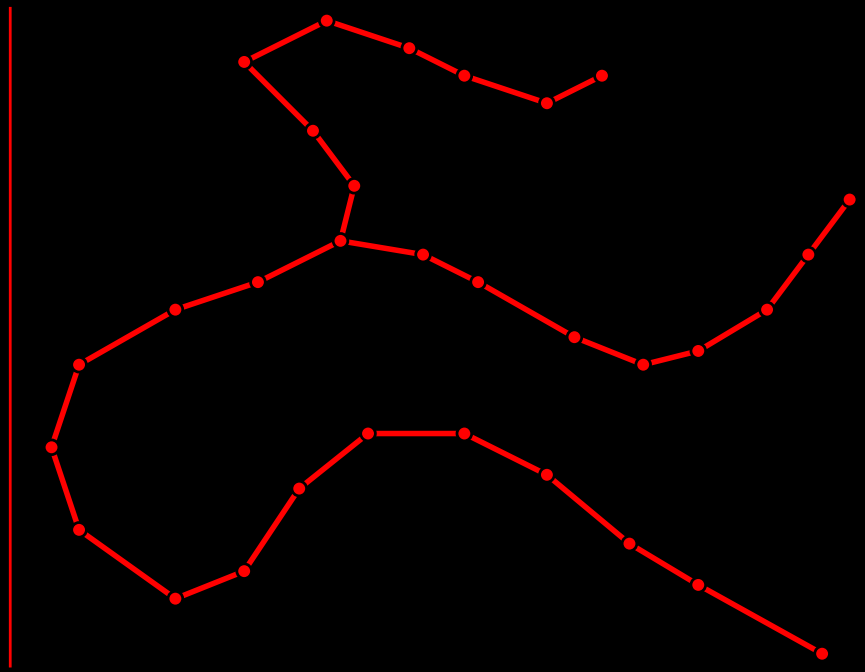

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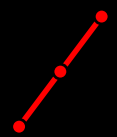

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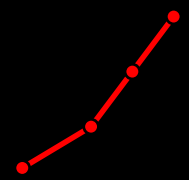

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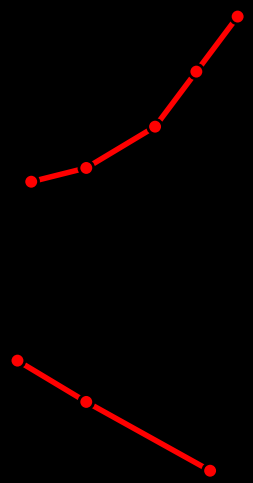

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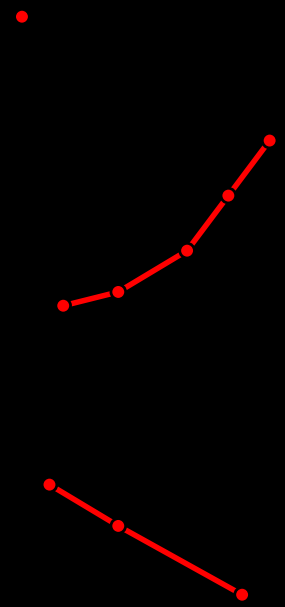

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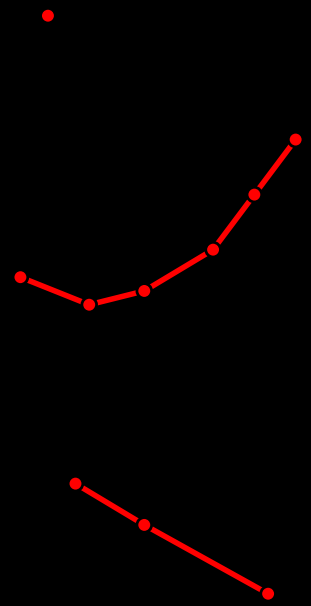

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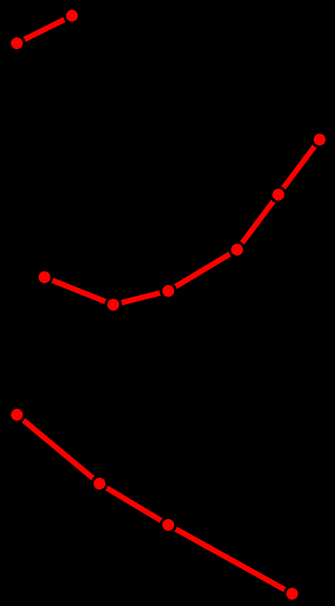

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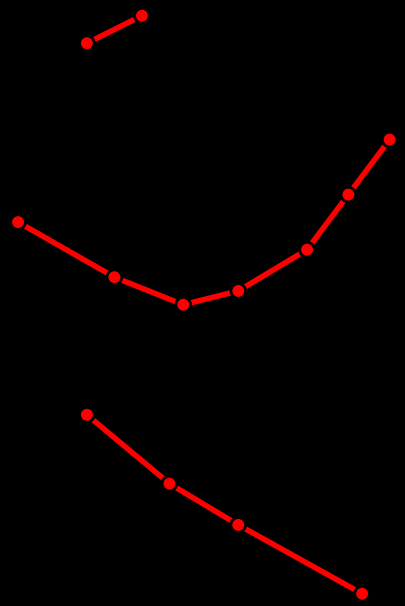

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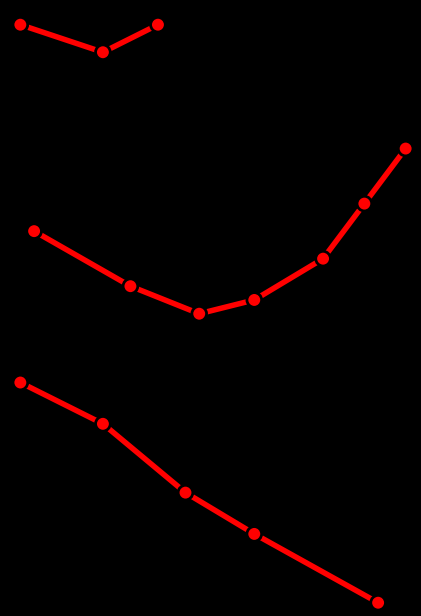

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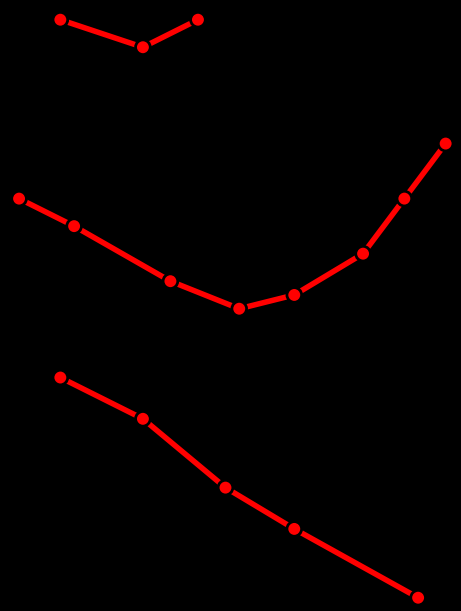

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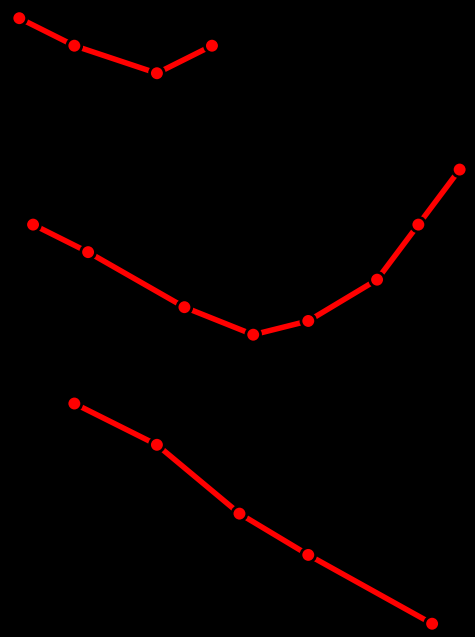

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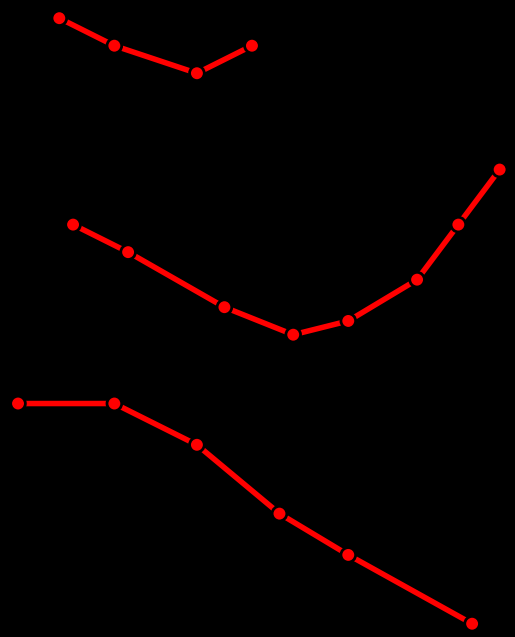

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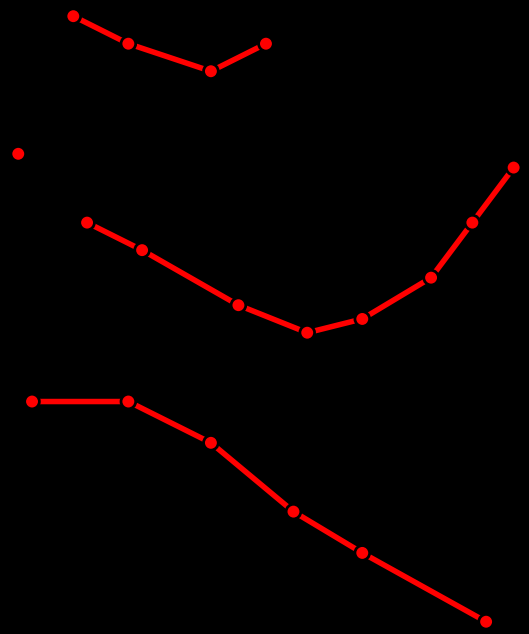

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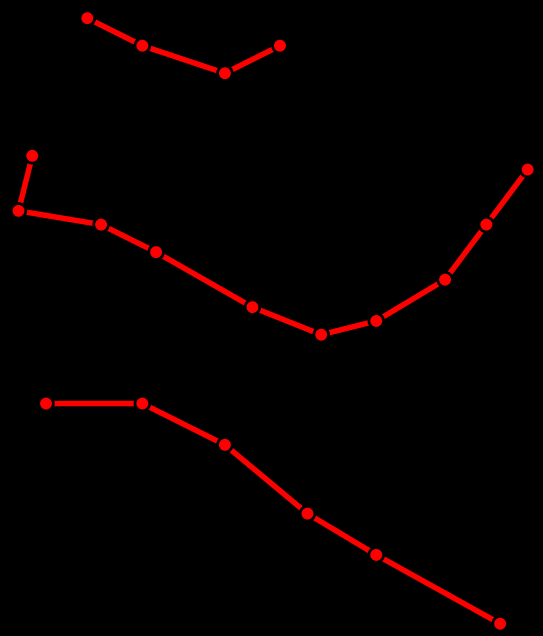

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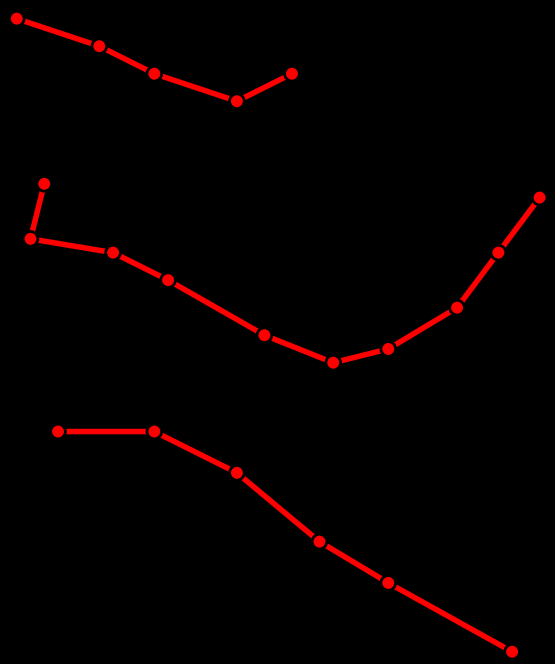

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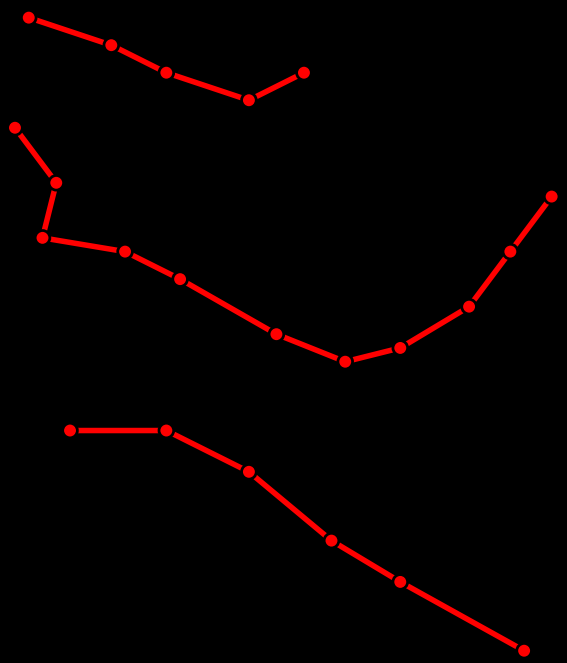

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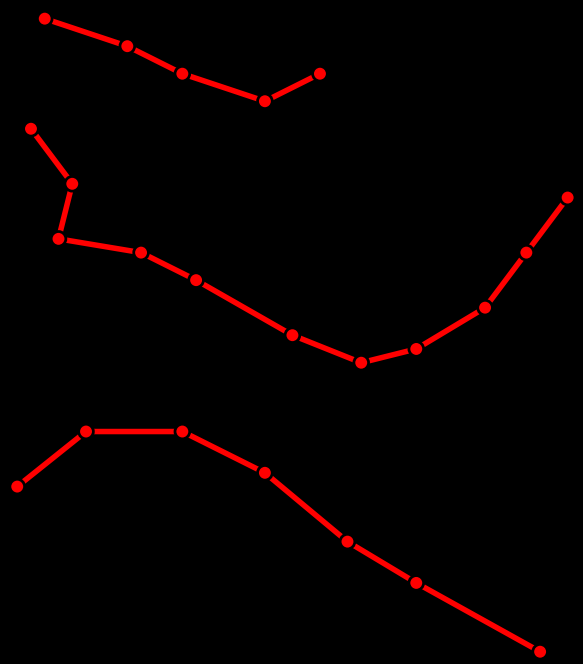

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Easily computable (if $\dim X$ is low; ambient space dim irrelevant).

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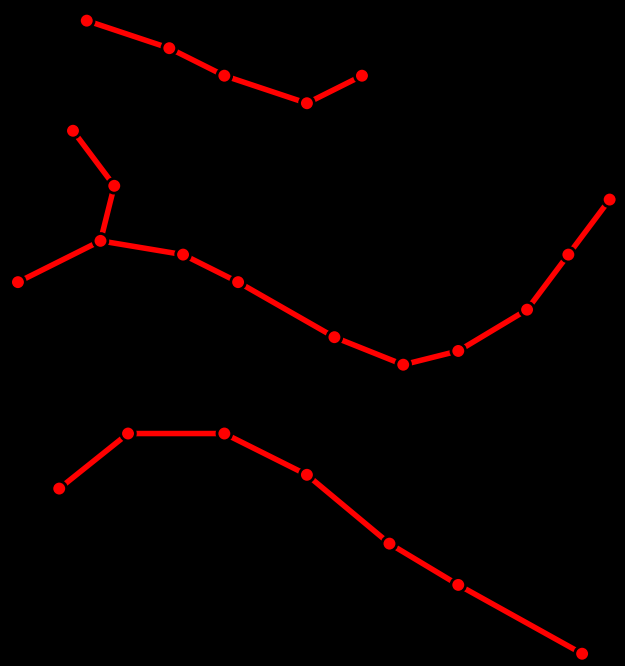

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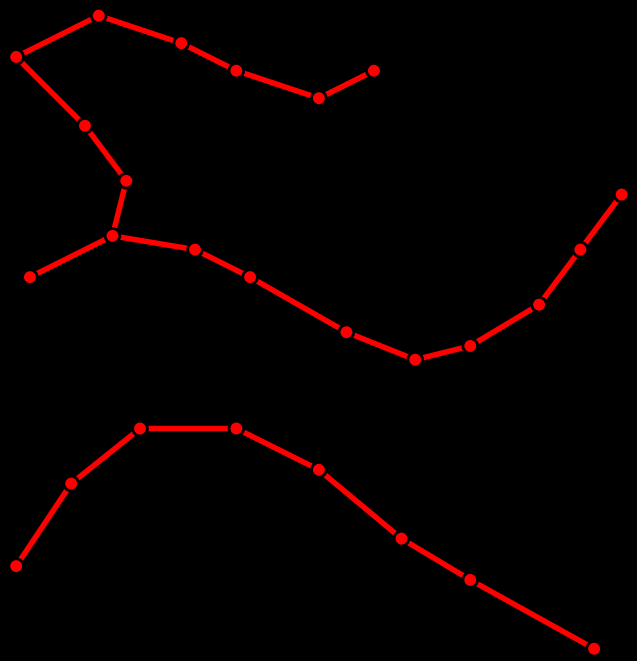

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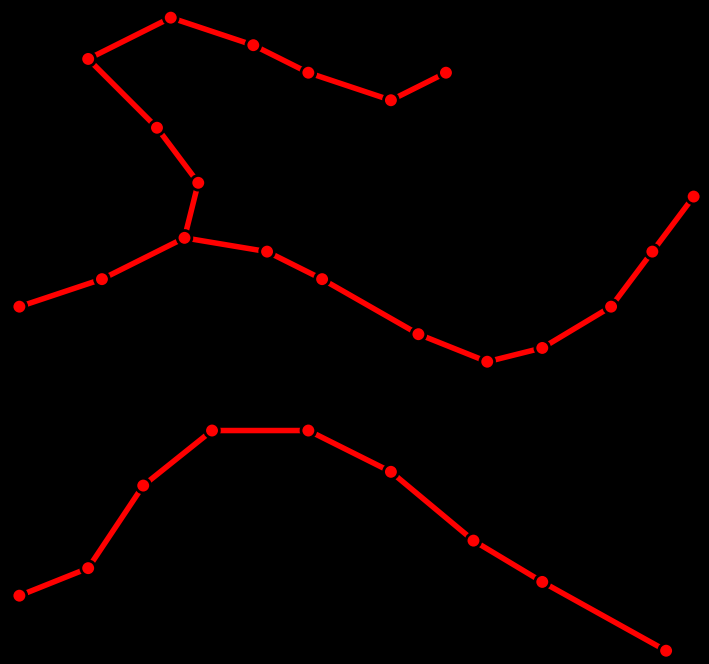

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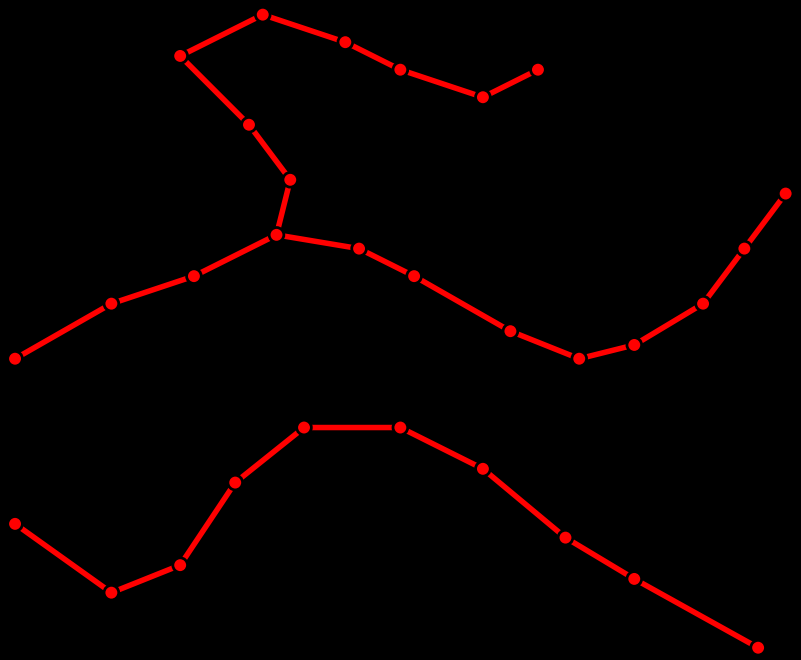

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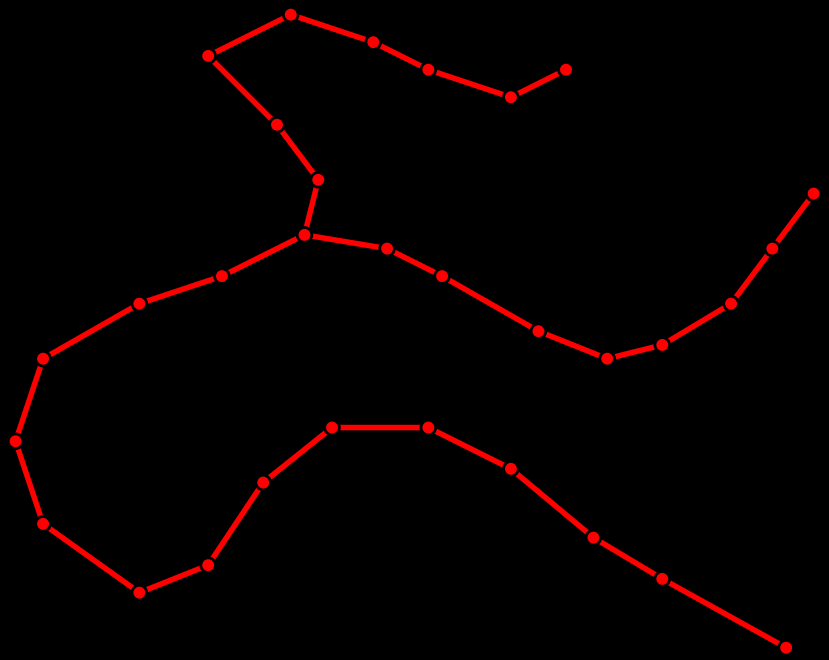

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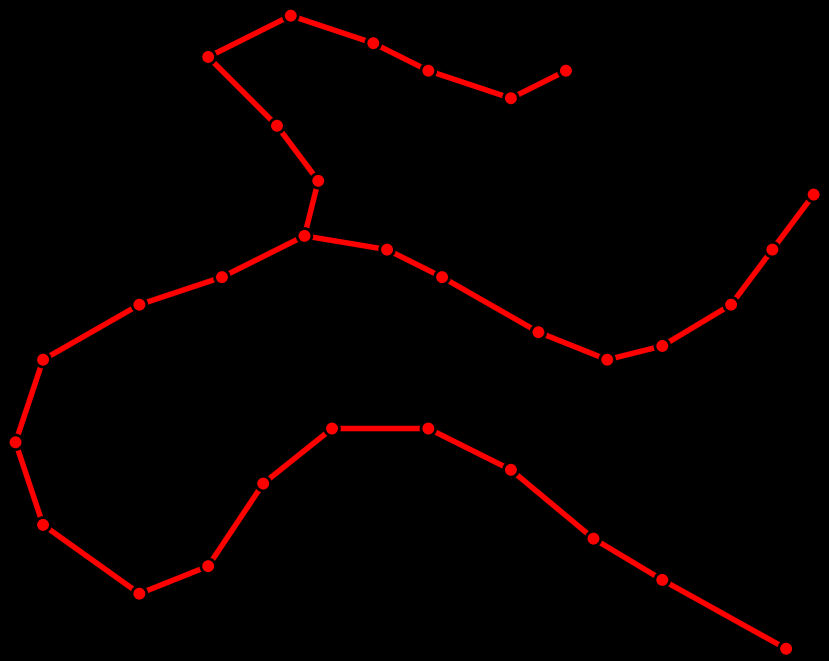

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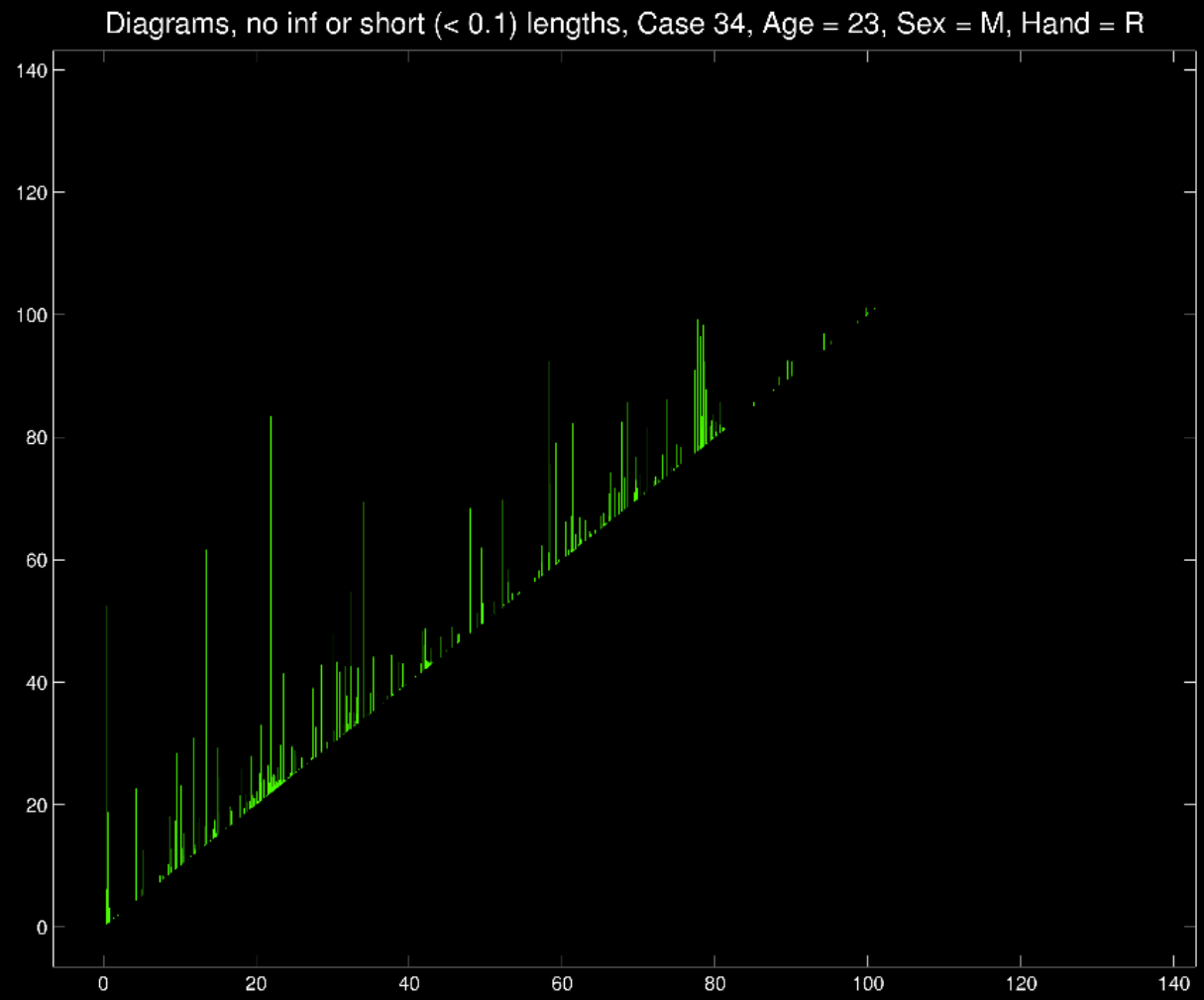
Bar codes

Data structure: 3D tree $\rightsquigarrow$ bar code / lace array / persistence diagram:



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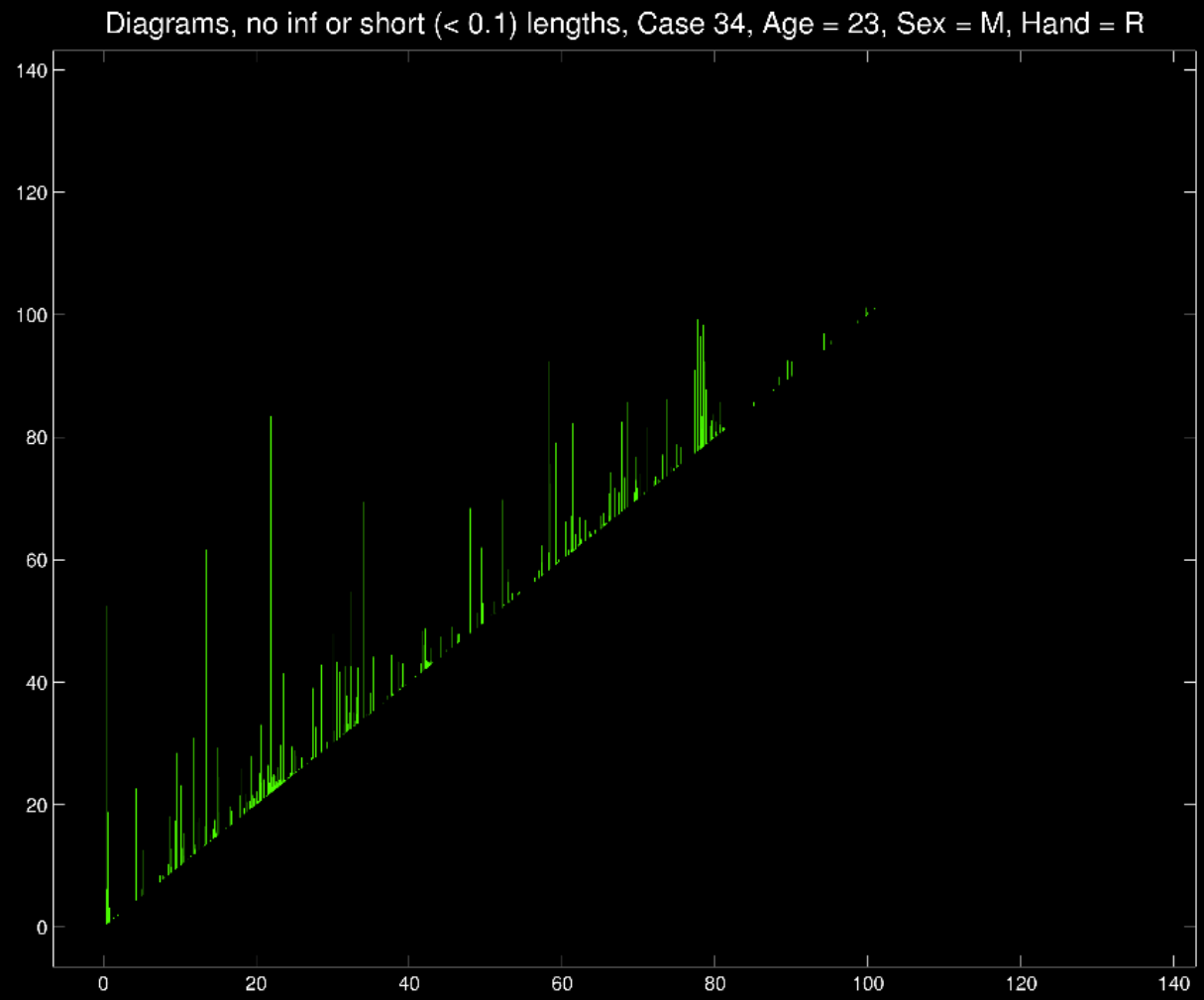

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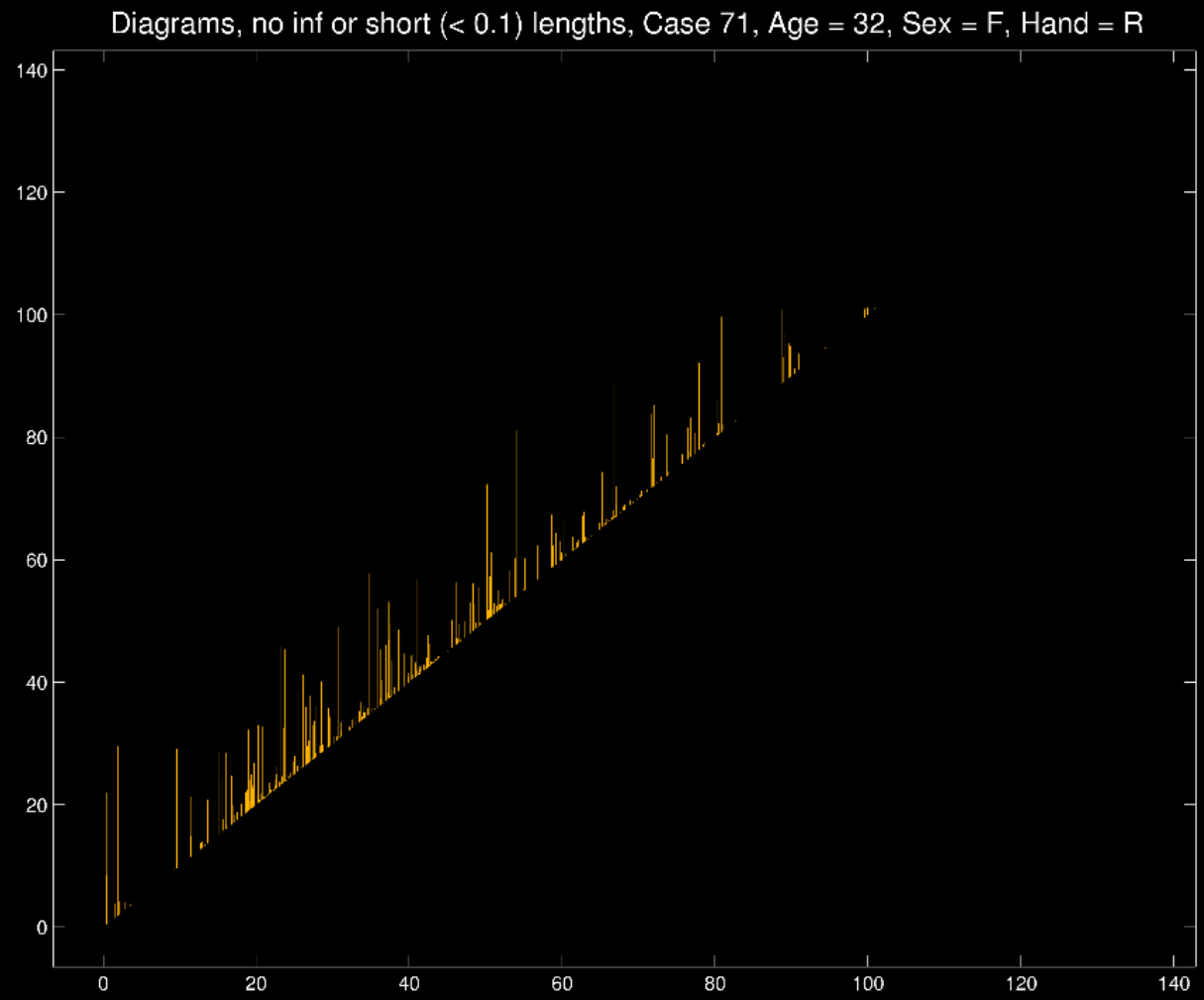

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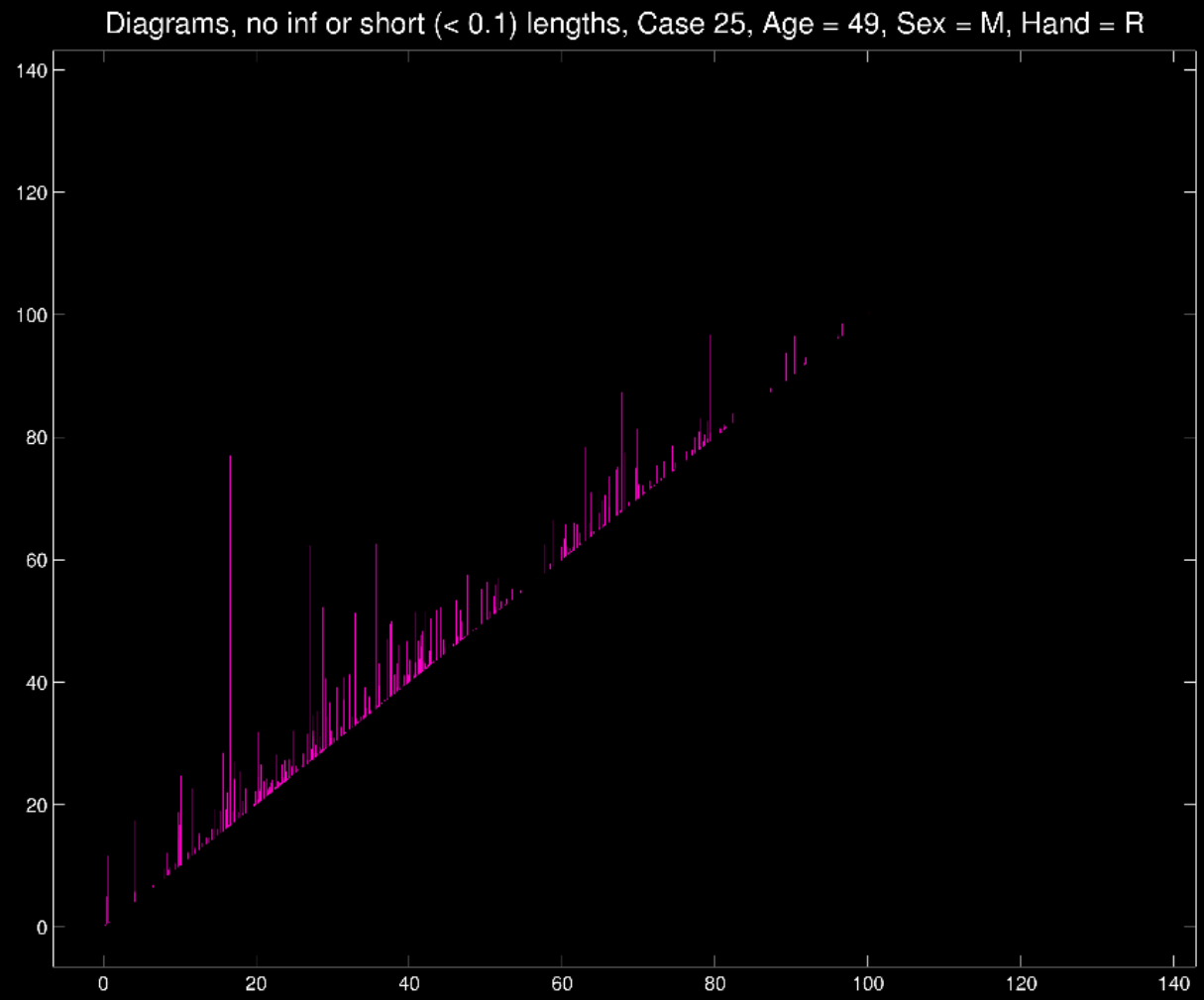

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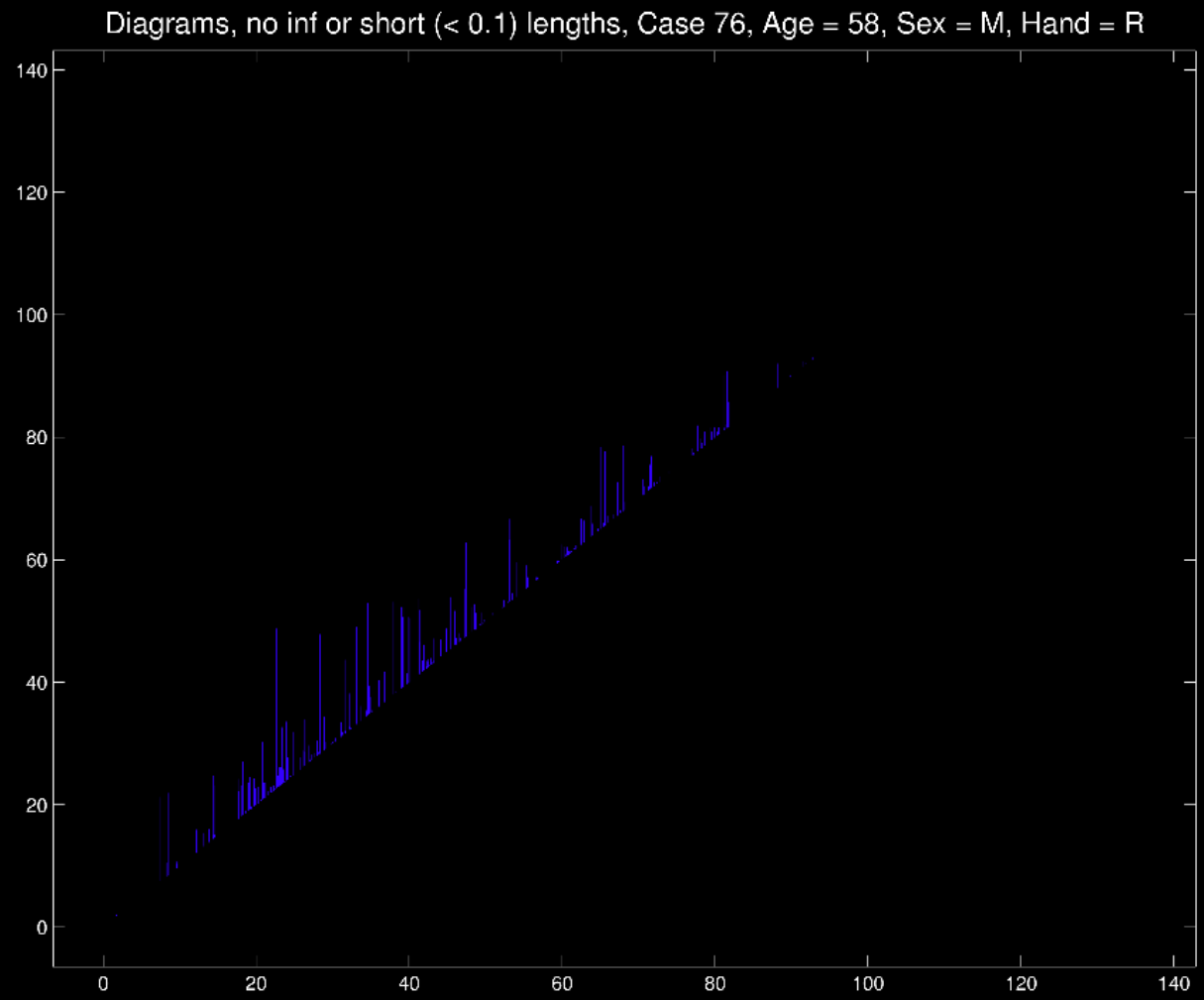

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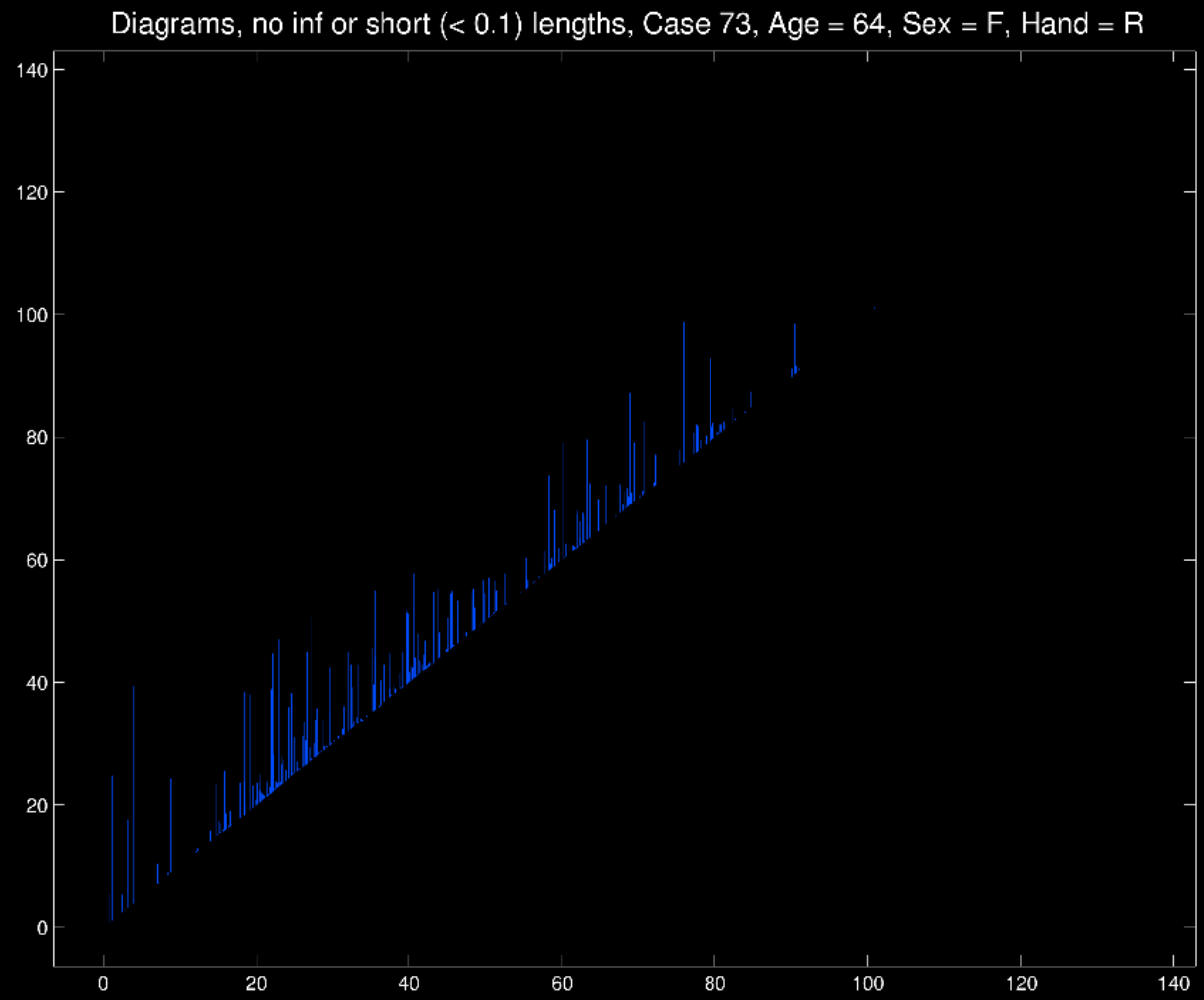

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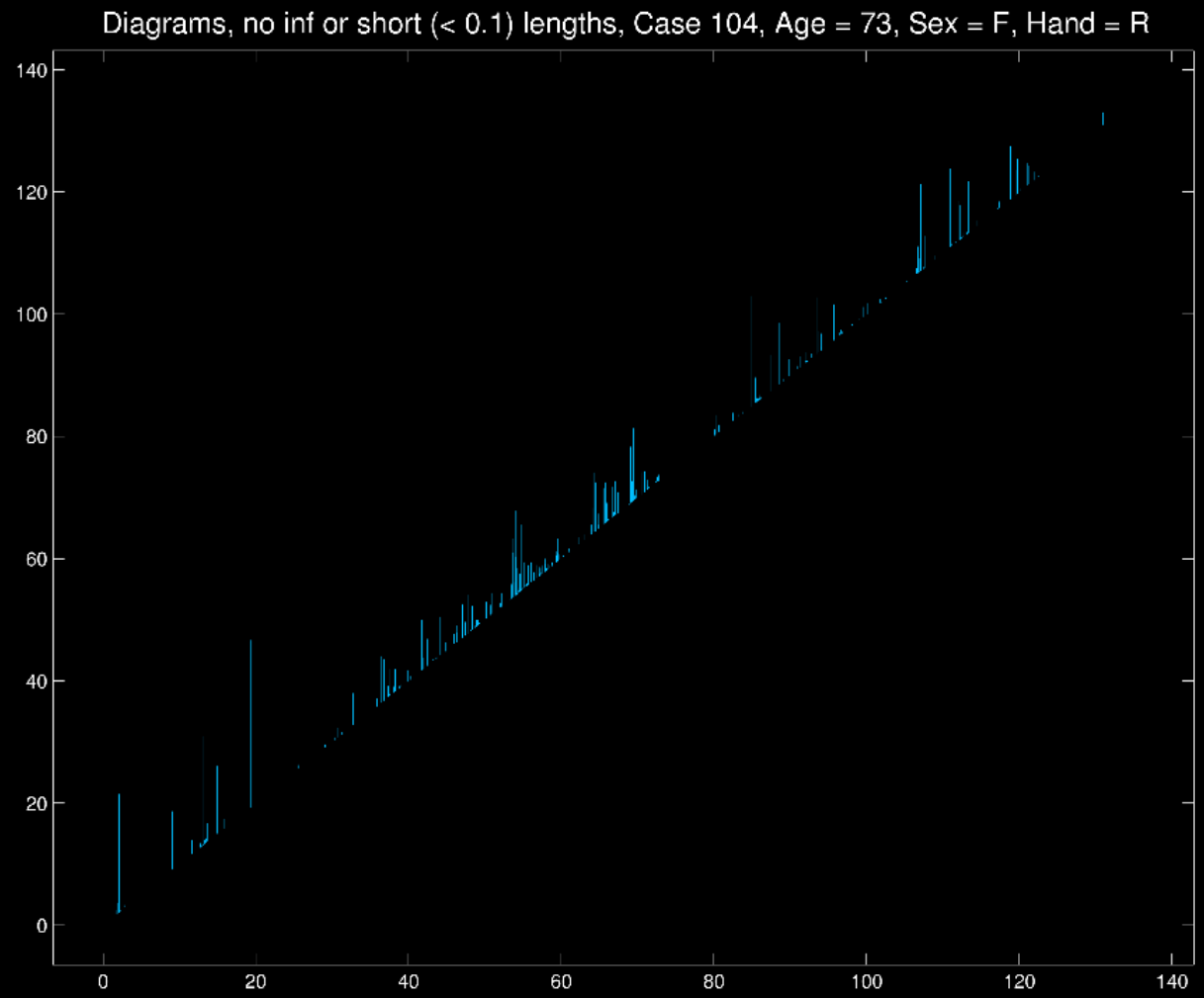

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Reduce to linear methods. 3D tree $\rightsquigarrow$ bar code $\rightsquigarrow$ vector in $\mathbb{R}^{100}$:

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Conclusions [Bendich–Marron–M.–Pieloch–Skwerer 2014]

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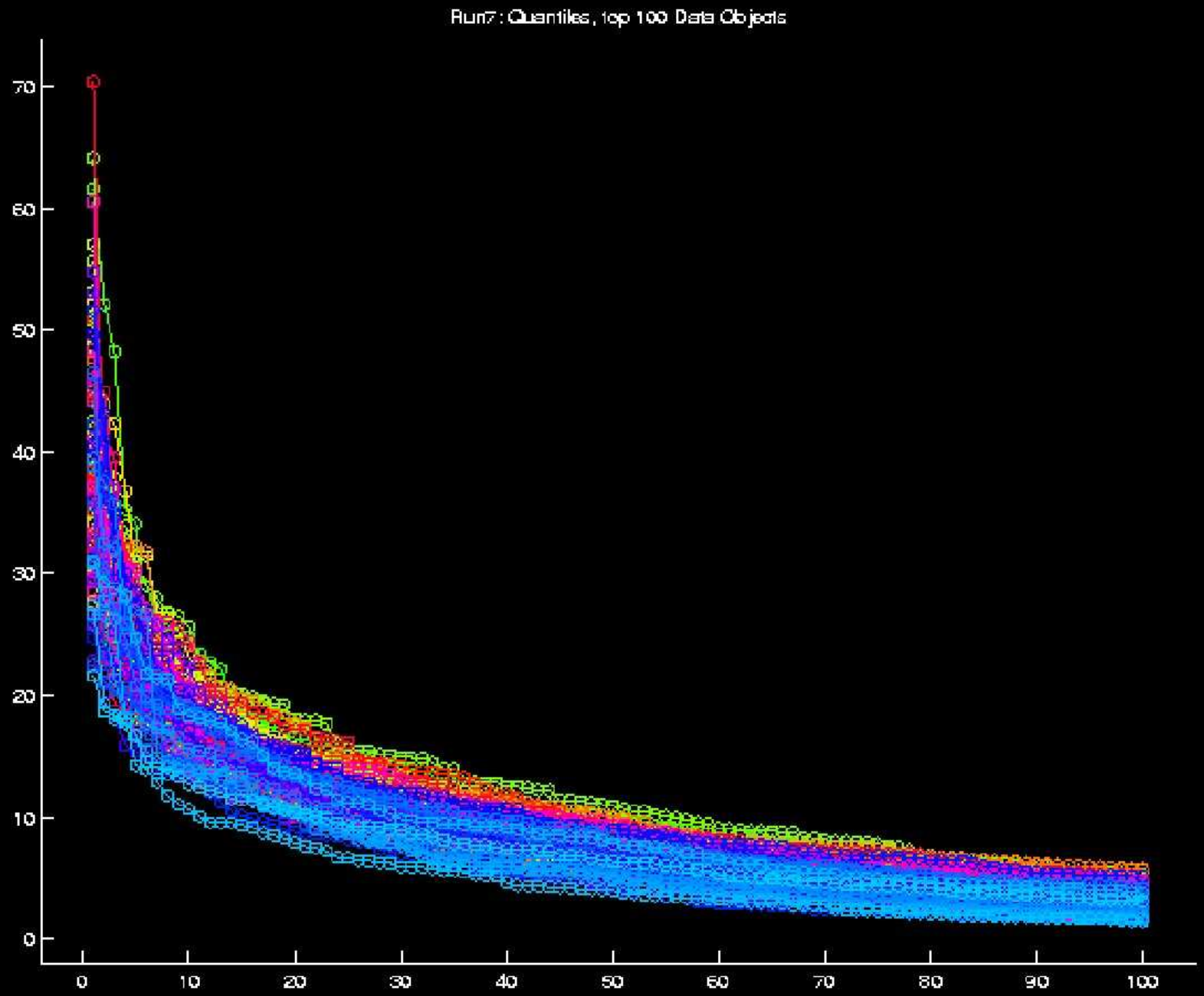
Moral. Persistent homology can topologically detect statistically significant geometric motifs

Top 100 bars


Run7: Quantiles, top 100 Data Objects
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
90
100

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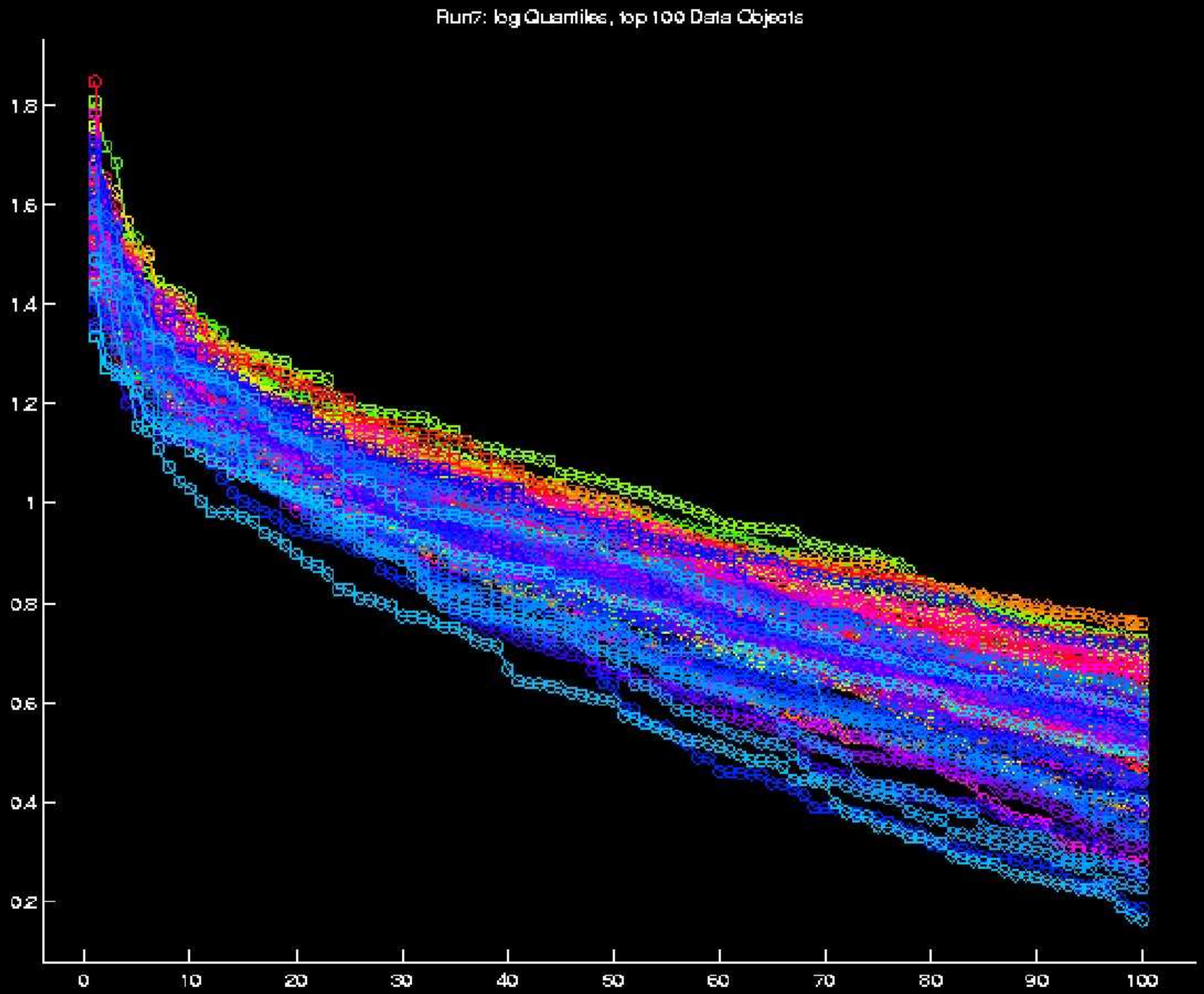
Top 100 bars: log scale



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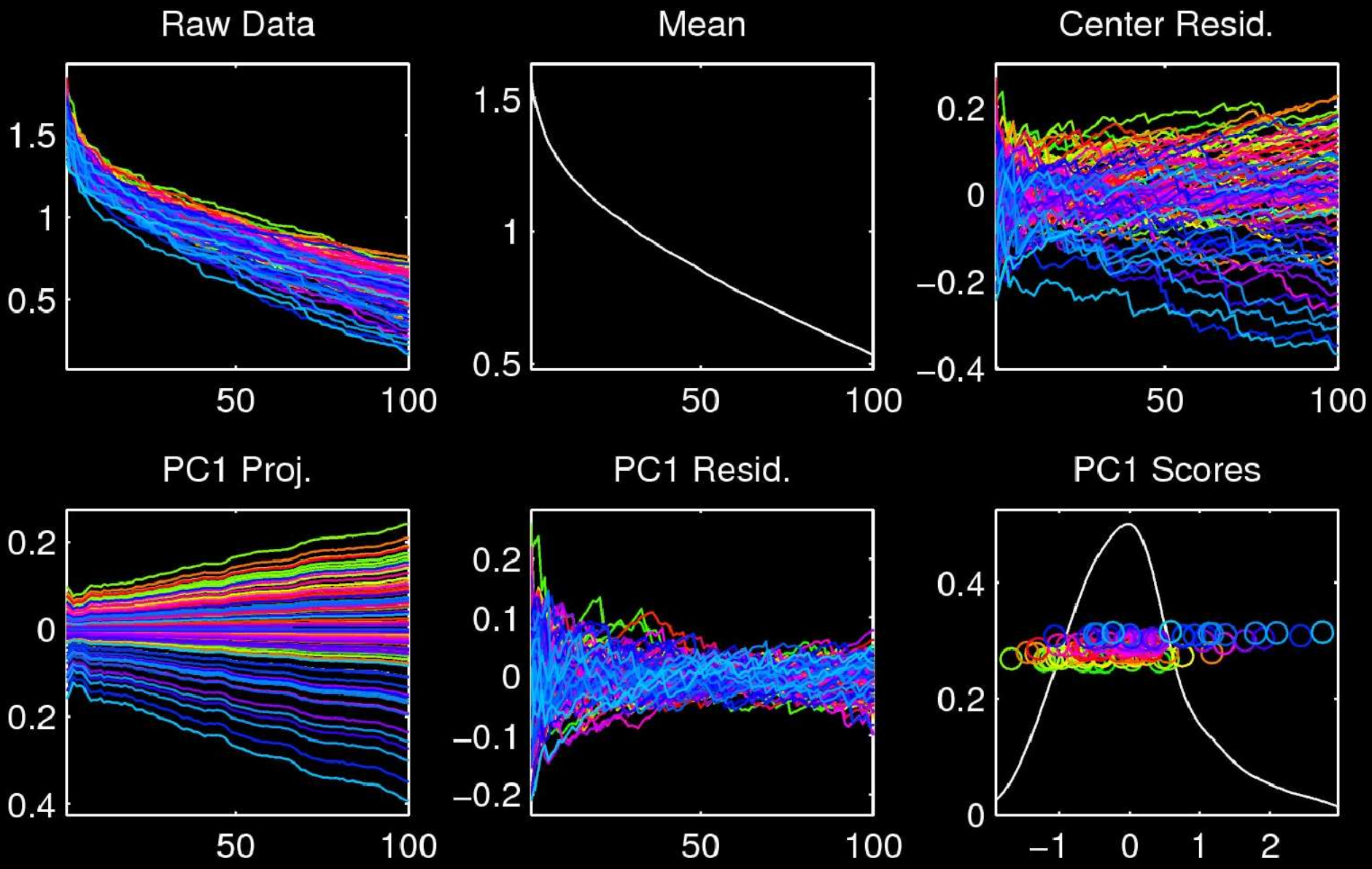
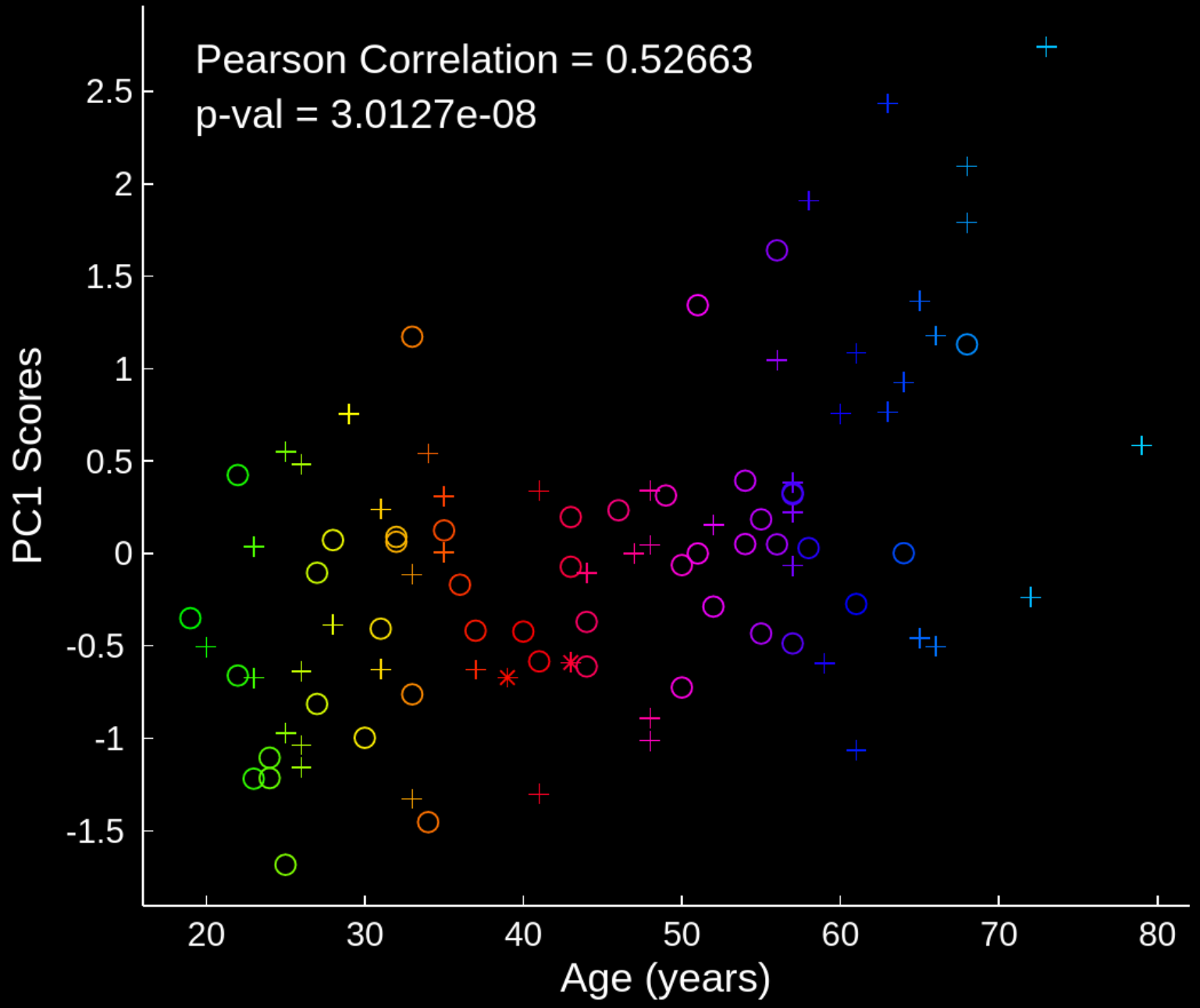
Age vs. PC1


Raw Data
Mean
Center Resid.
PC1 Proj.
PC1 Resid.
PC1 Scores
1.5
1
0.5
50
100
0.2
0
−0.2
−0.4
0.1
0.4
−1
2

Age vs. PC1


Pearson Correlation = 0.52663
p-val = 3.0127e-08
PC1 Scores
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
20
30
40
50
60
70
80
Age (years)

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Reflections on persistent homology

Where did the best correlation occur?

- How did we choose top 100 bar lengths?
- What choices yield the best correlation? Why?

Old persistent homology mantra: most significant features

- are "biggest"
- live "far from the diagonal" in bar codes.

For brain artery trees

- Not surprising that very short bars $\leftrightarrow$ noise, although in other studies they might not.
- While biggest features are important,
- they hinder strength of correlation.

Lessons

- Importance $\not\Rightarrow$ significance for geometric features.
- Persistent homology can detect significant features lying between important and noise.

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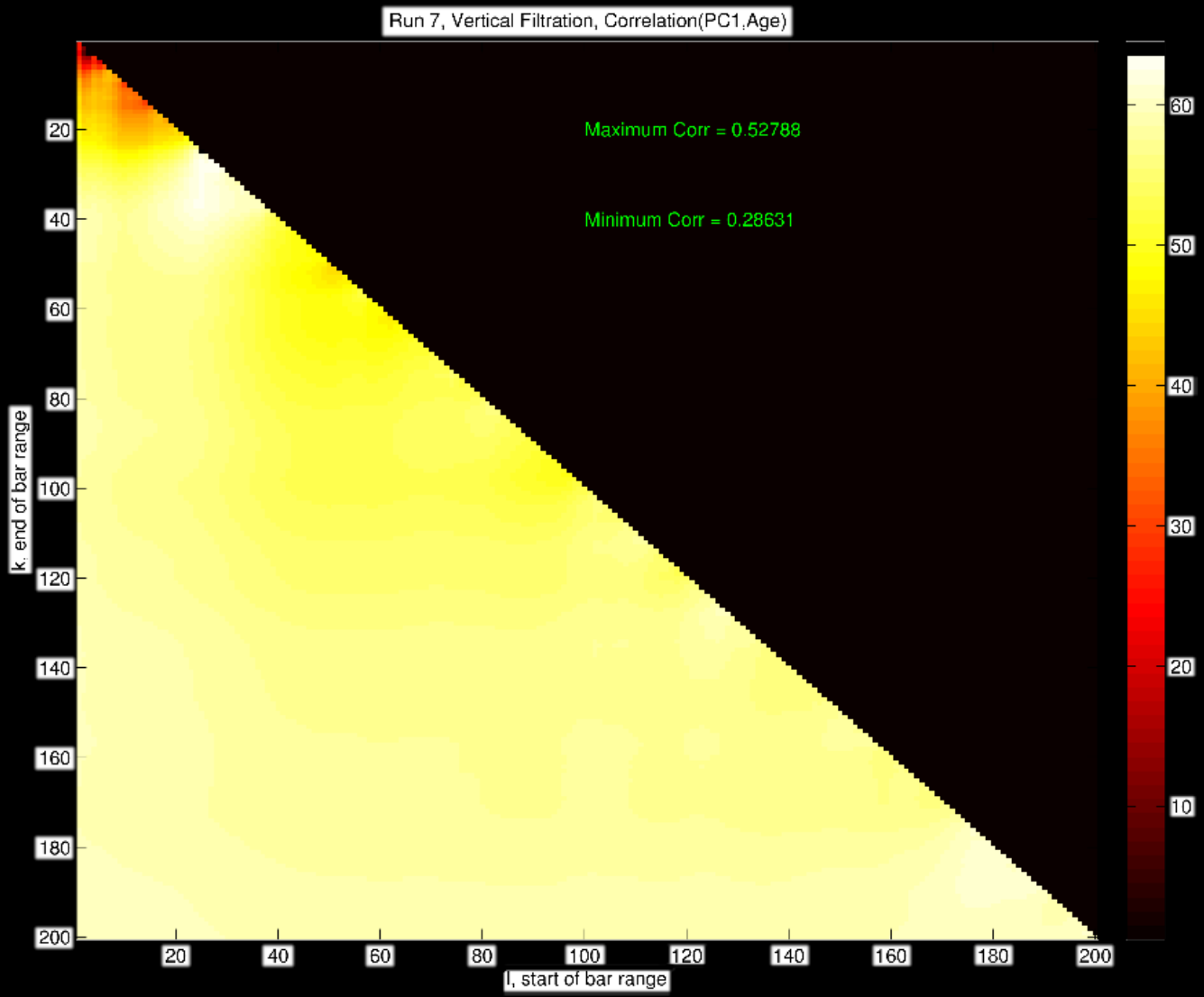

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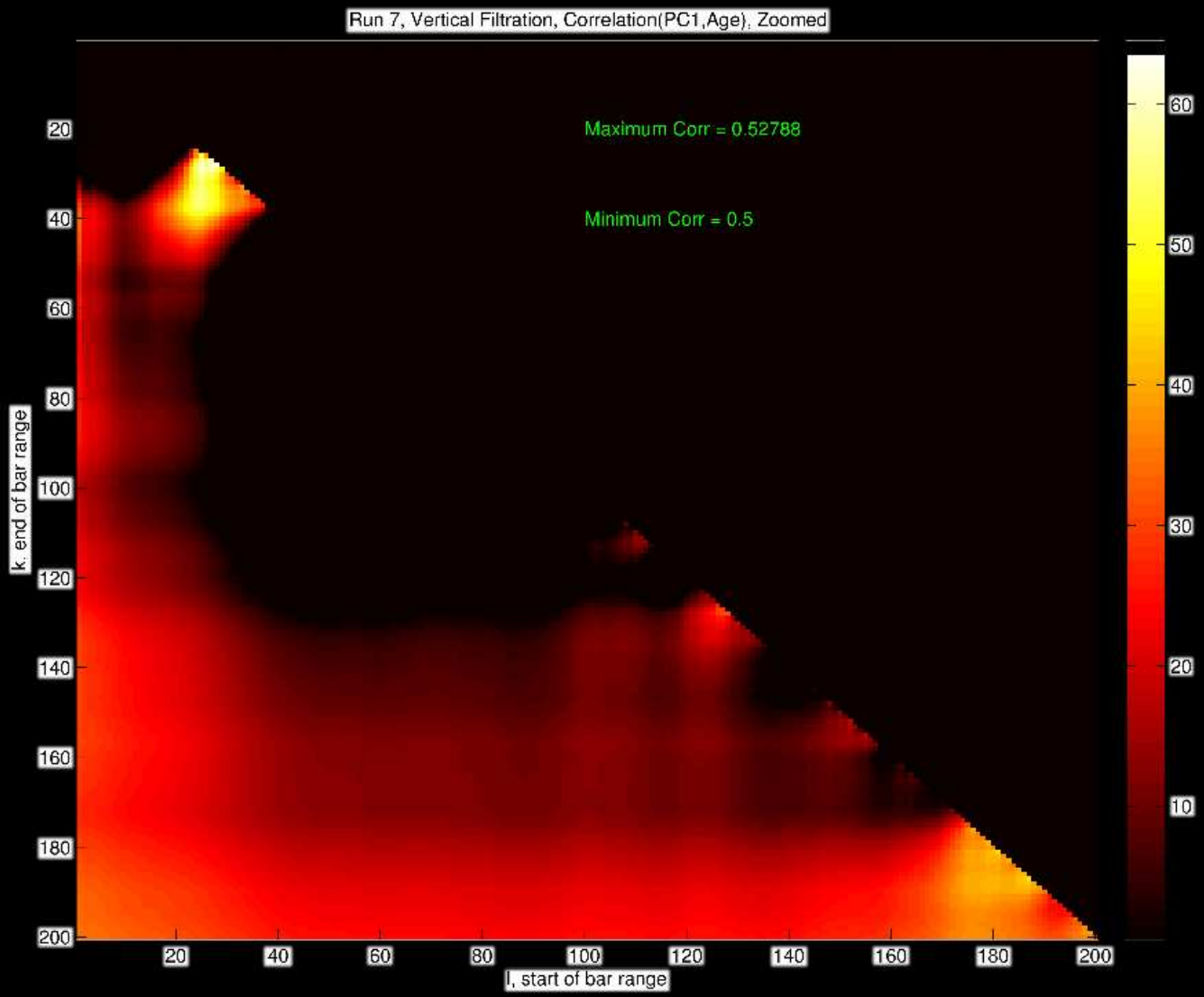

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Looking forward

Implementation

- single preprocessing step for many multiPH computations; e.g., fly wings
- Lebesgue distance computations: no sampling for Riemann integration

Invariants

- E.g., what could "top 100 bar lengths" mean in multipersistence?
- E.g., boundaries of up- or downsets $\rightsquigarrow$ "highly persistent" elements

Real L^p distances [Bubenik–Scott–Stanley 2023], [Skraba–Turner 2023], [Bjerkevik–Lesnick 2021]

- integer parameters: match pairs of generators
- real parameters: sums $\to \infty$ with finer discrete approximation
- instead: use L^p distances between boundaries of up- and downsets...
- ...from corresponding associated primes (same history or mortality type)

Relative homological algebra

- resolve using upsets and/or downsets
- Conj: $\mathbb{R}^n$-modules have upset resolutions of length at most $n-1$.
- Compare [Geist–M.– 2023]: $\Bbbk[\mathbb{R}^n_+]$ has global dimension $n+1$.

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- E.g., what could "top 100 bar lengths" mean in multipersistence?
- E.g., boundaries of up- or downsets $\rightsquigarrow$ "highly persistent" elements

Real L^p distances [Bubenik–Scott–Stanley 2023], [Skraba–Turner 2023], [Bjerkevik–Lesnick 2021]

- integer parameters: match pairs of generators
- real parameters: sums $\to \infty$ with finer discrete approximation
- instead: use L^p distances between boundaries of up- and downsets...
- ...from corresponding associated primes (same history or mortality type)

Relative homological algebra

- resolve using upsets and/or downsets
- Conj: $\mathbb{R}^n$-modules have upset resolutions of length at most $n-1$.
- Compare [Geist–M.– 2023]: $\Bbbk[\mathbb{R}^n_+]$ has global dimension $n+1$.

Looking forward

Implementation

- single preprocessing step for many multiPH computations; e.g., fly wings
- Lebesgue distance computations: no sampling for Riemann integration

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Thank You