Algebra for topology in biology and statistics

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and Department of Statistical Science

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ongoing mathematics with Justin Curry and Ashleigh Thomas (Duke)

and biology with David Houle (Florida State, Biology)

Interactions between Algebra and the Sciences

Max Planck Institut für Mathematik
in den Naturwissenschaften

27 May 2017

Outline

1. Biology
2. Data
3. Questions
4. Statistics
5. Algebra
6. Fly wings
7. Biological background
8. Persistent homology
9. Poset modules
10. Encoding persistence modules
11. Fringe presentation
12. Topology of probability distributions
13. Future directions

What kinds of biology?

Geometric datasets and data objects arise naturally in biological sciences:

- medicine
- neuroscience
- botany
- ecology
- systems biology: organisms as collections of interacting units
  - metabolic pathways
  - cell signaling networks
- systematics: history of speciation
- evolutionary biology: mechanisms of selection and speciation
- developmental biology: embryology, cell differentiation, growth
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Note. We guide biologists to relevant techniques for their data and questions $\Rightarrow$ crucial to

- understand data on biologists' terms
- be aware of available statistical or mathematical methods

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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    - any bunch of isolated points in $\mathbb{R}^n$ (!), especially for $n \gg 0$

Networks

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- metabolic
- regulatory (genetic)
- phylogenetic
- ecological
- physical: plant roots, neuronal (dendritic)

Points in high dimension, e.g. genetic SNP profiles for personalized medicine

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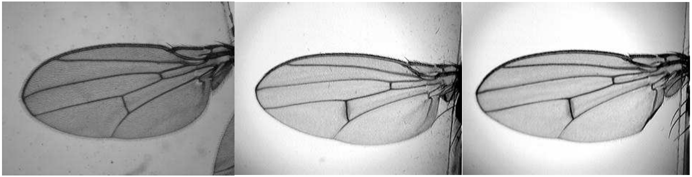
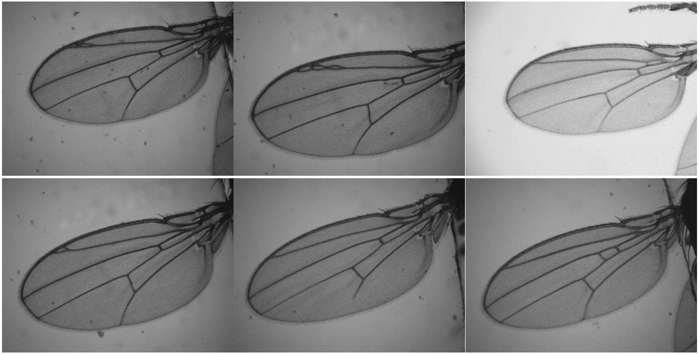
Fruit fly wings

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



Topologically abnormal veins:



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A. apoplanos

courtesy Elen Oneal

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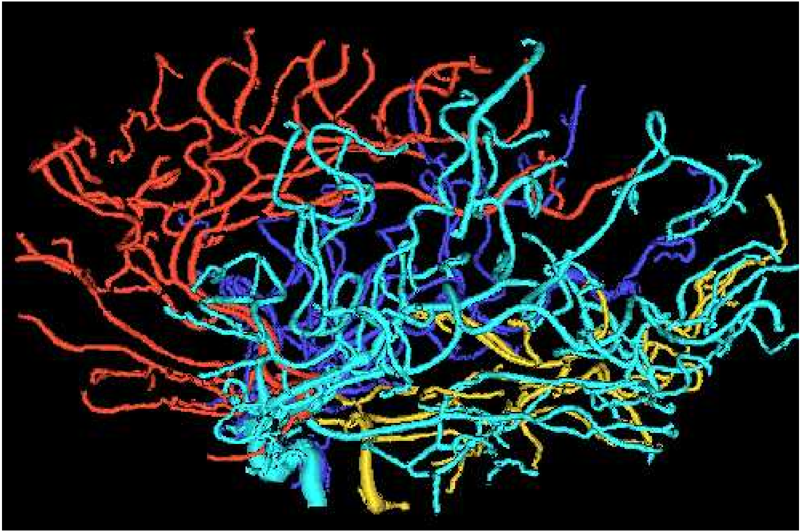

[Bullitt and Aylward, 2002]

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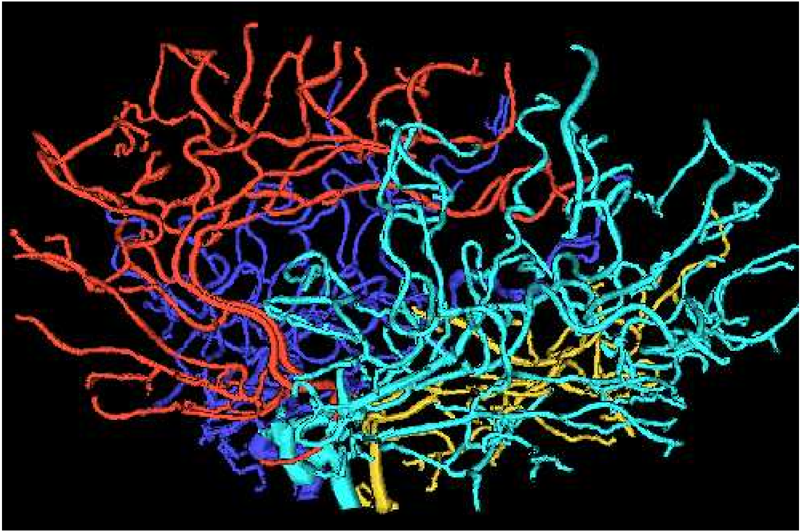

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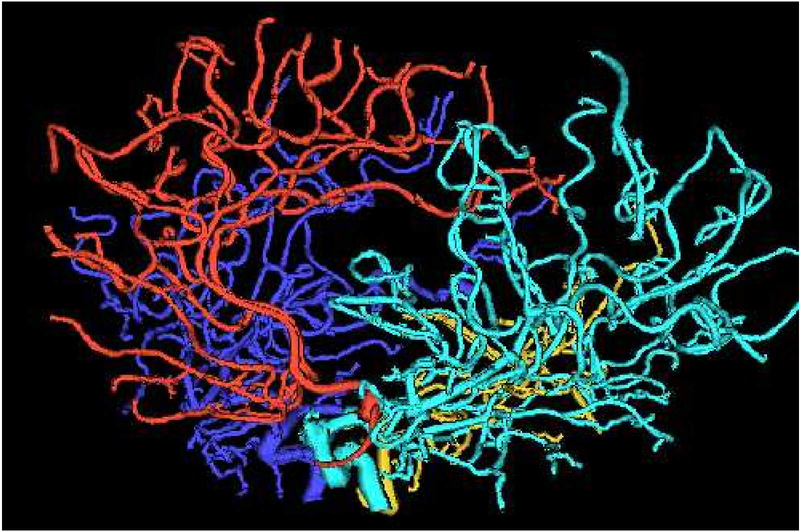

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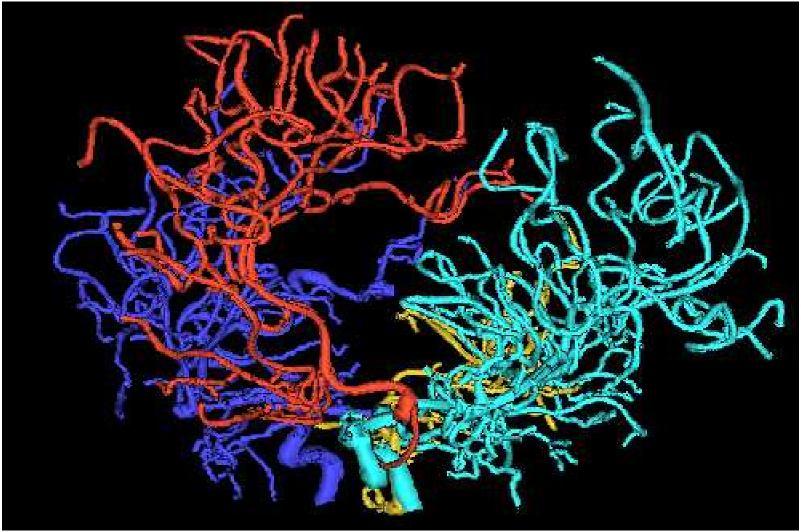

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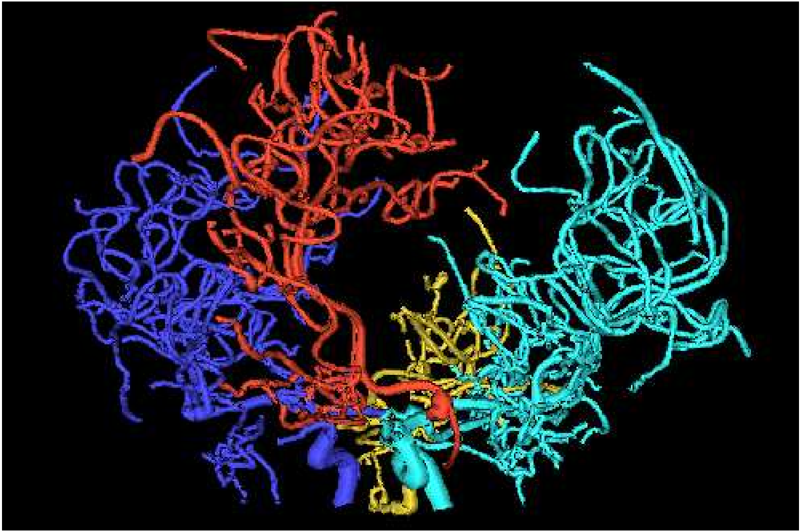

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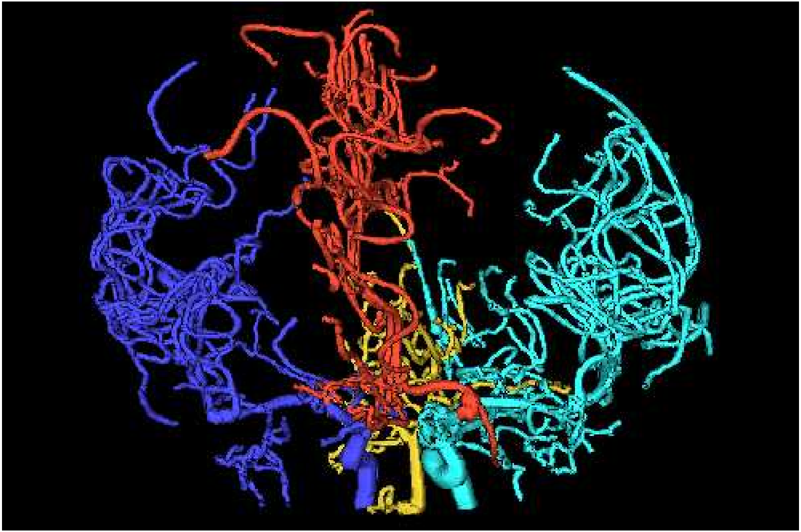

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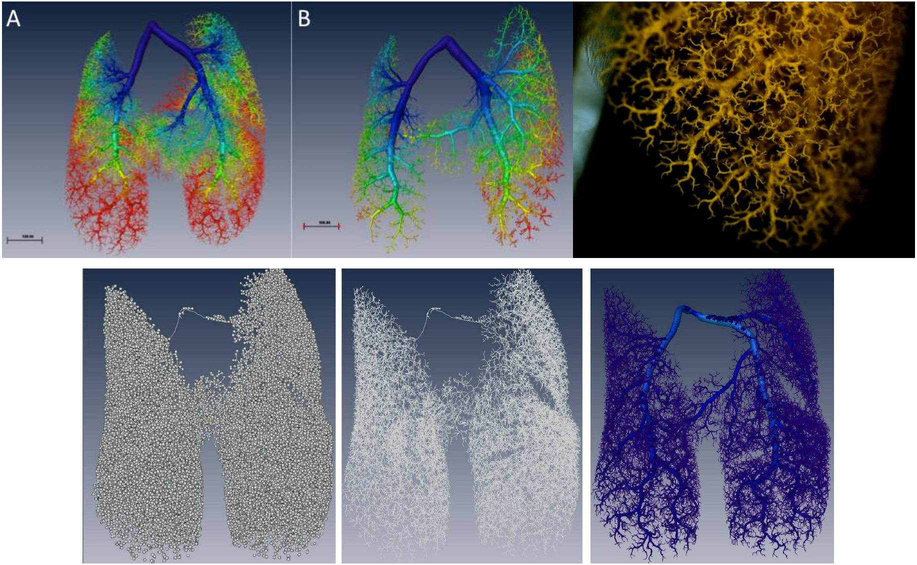
Lung vessels (CDH study)



courtesy Sean McLean

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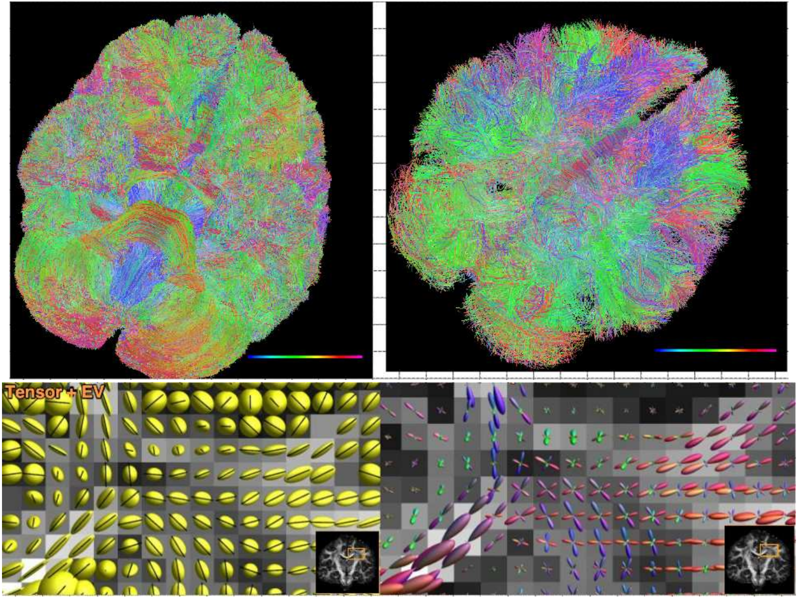
Streamlines from Diffusion Tensor Imaging



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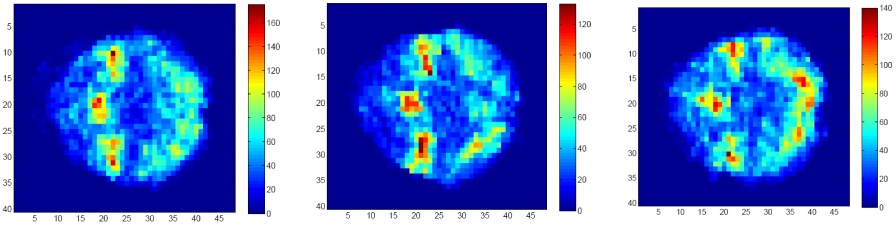
fMRI



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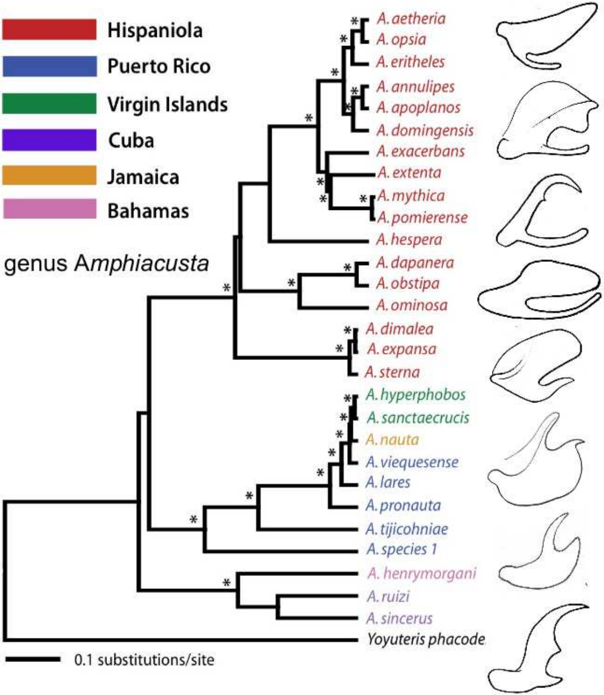

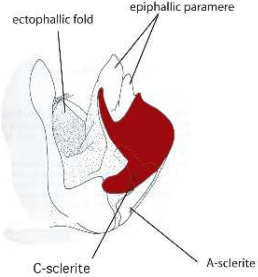

From Oneal, Otte & Knowles, 2010

Drawings by Dan Otte

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What kinds of questions?

Discover statistical trends in geometric structures

- plant roots, neurons: classification
- phylogenetic trees: reconstruct, estimate
- biochemical networks:
  - parameter estimation (rate constants)
  - stability or (multi)stationarity, especially when independent of parameters
- points in $\mathbb{R}^n$: ordinary statistics, or any invariant, e.g., homology
- principal bundles to explain aperiodicity: model selection
- fMRI: classification
- fiber tracts: network estimation or model selection
- brain arteries: age, sex, handedness; eventually: stroke tendency, tumor
- sclerites (or any morphometric data): phylogenetic relationships
- lung vessels: well, anything [currently in conversation]
- fly wings: we'll get to that

Geometric reconstruction

- of space from neural codes
- of 3D images from 2D

What kinds of statisticians?

Those who deal with

- geometric data, such as brain scans—either 3D or 4D
- graph-theoretical data
- high-dimensional data, particularly with low sample size
- data from nonlinear spaces: angles, shapes, phylogenetic trees, . . .

Standard tools

- lots of highly (spatially or temporally) correlated variables (# variables can be in the millions or higher order of magnitude for fMRI)
- linear regression: PCA = best-fit linear subspace
- classification schemes: *k*-nearest neighbor, support vector machines, . . .

Newer tools

- manifold learning
- persistent homology
- nested spheres

What kinds of algebra?

Methods based on

- algebraic and differential geometry
  - spaces of phenotypes or phenotype summaries
    - configuration spaces of points (“shape spaces”)
    - moduli spaces of modules
  - grassmannians
  - model parameters satisfying given constraints [Conradi]
- polyhedral or tropical geometry
  - spaces of trees [Bernstein]
  - -opes and -hedra of various sorts (e.g. genotope)
- monomial and binomial algebra
  - neural rings [Lienkaemper]
    related to [Martini]: realizability of combinatorial configurations
  - toric dynamical systems
  - probability simplices and subvarieties [Kubjas]
- topology and combinatorics
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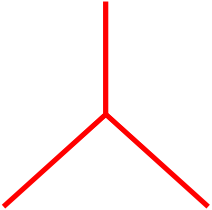
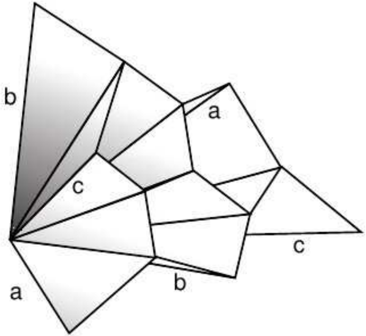
Pictures of tree spaces



$\mathcal{T}_3$



$\mathcal{T}_4$
from [BHV 2001]

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Methods based on

- algebraic and differential geometry
  - spaces of phenotypes or phenotype summaries
    - configuration spaces of points (“shape spaces”)
    - moduli spaces of modules
  - grassmannians
  - model parameters satisfying given constraints [Conradi]
- polyhedral or tropical geometry
  - spaces of trees [Bernstein]
  - -opes and -hedra of various sorts (e.g. genotope)
- monomial and binomial algebra
  - neural rings [Lienkaemper]
    related to [Martini]: realizability of combinatorial configurations
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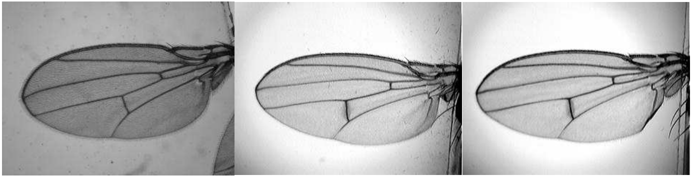
especially computational aspects

Fruit fly wings

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



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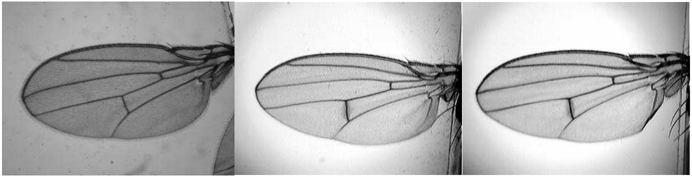
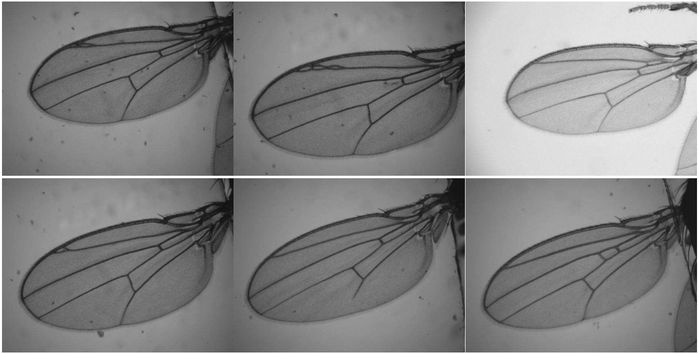
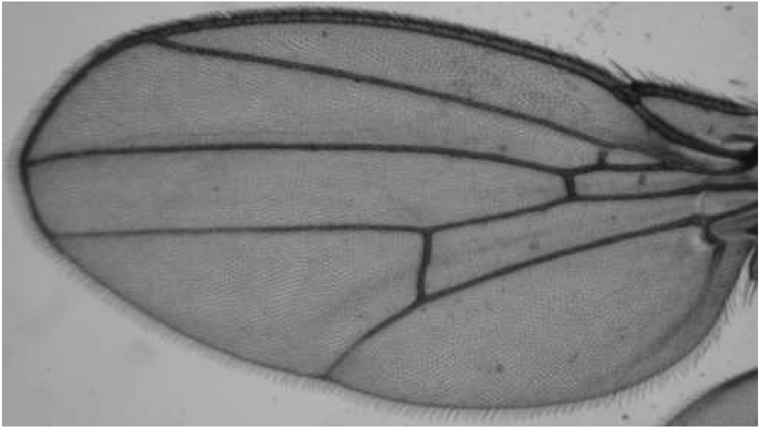


Topologically abnormal veins:



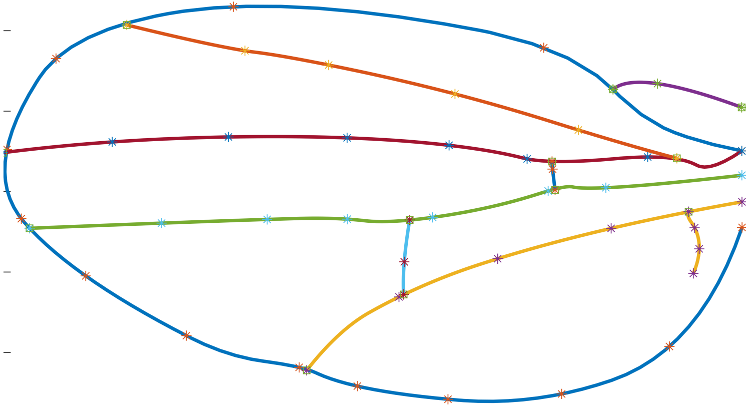
Fruit fly wings

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

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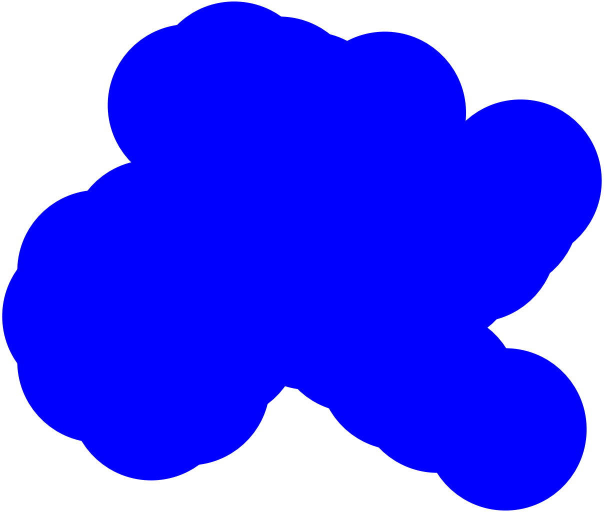
Example: expanding balls



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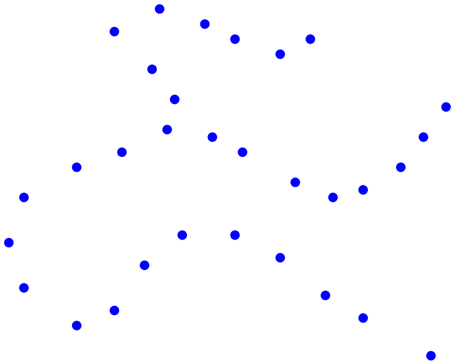

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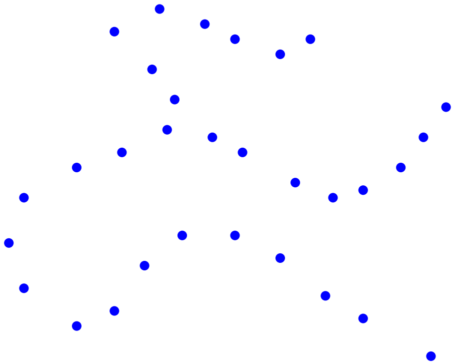

$\dim(H_0) = 31$

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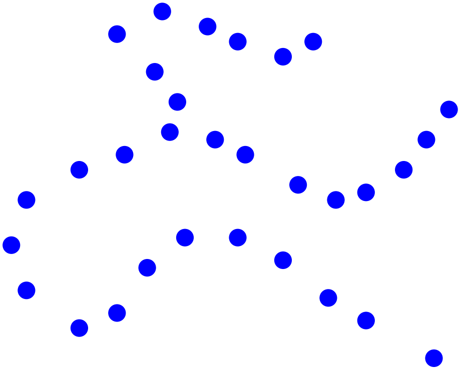

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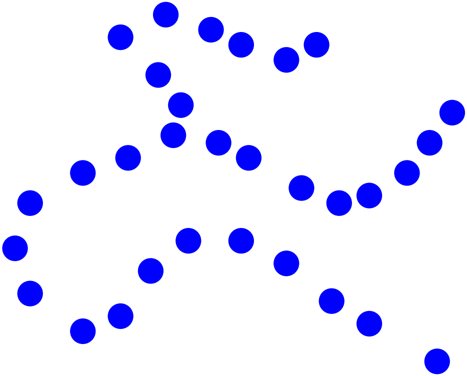

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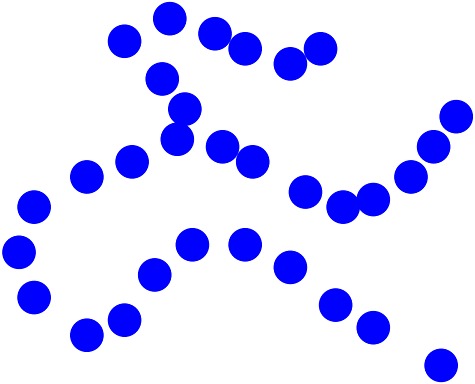
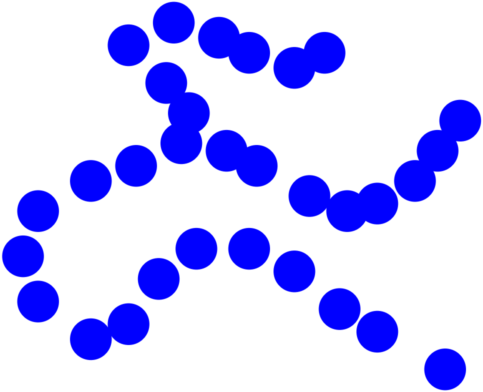


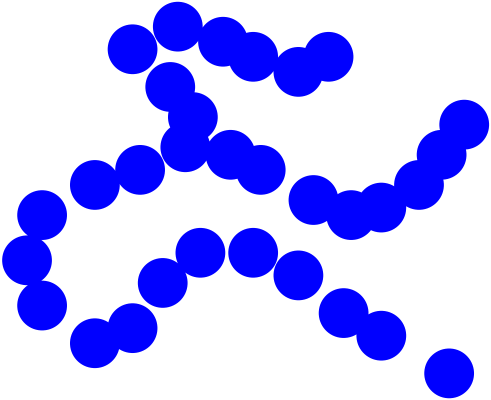
$\dim(H_0) = 26$

Example: expanding balls



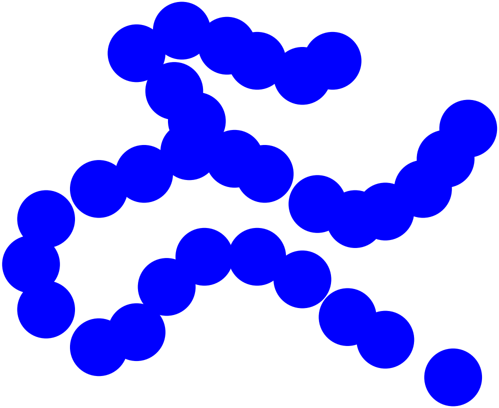
$\dim(H_0) = 21$

Example: expanding balls



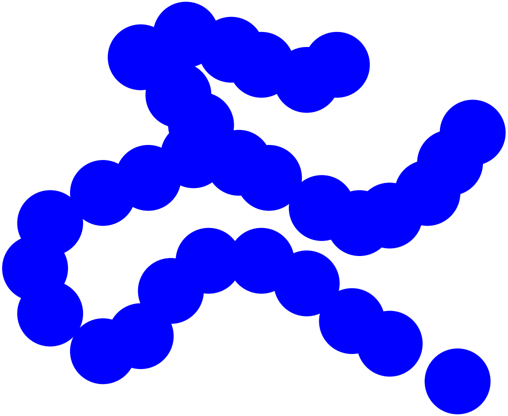
$\dim(H_0) = 12$

Example: expanding balls



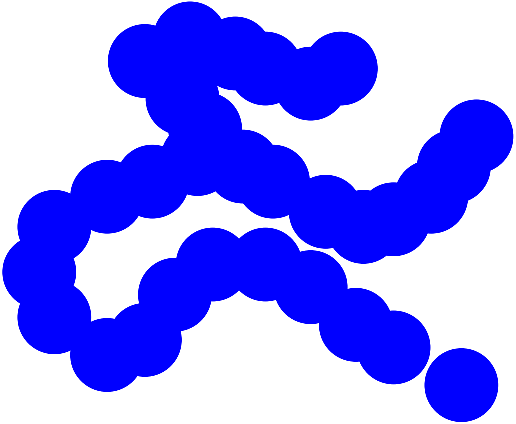
$\dim(H_0) = 6$

Example: expanding balls



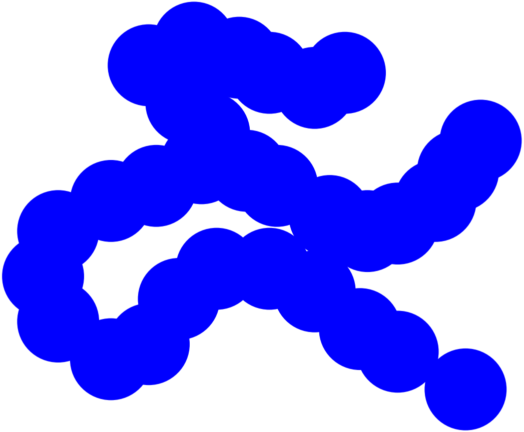
$\dim(H_0) = 2$

Example: expanding balls



$\dim(H_0) = 2$

Example: expanding balls



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

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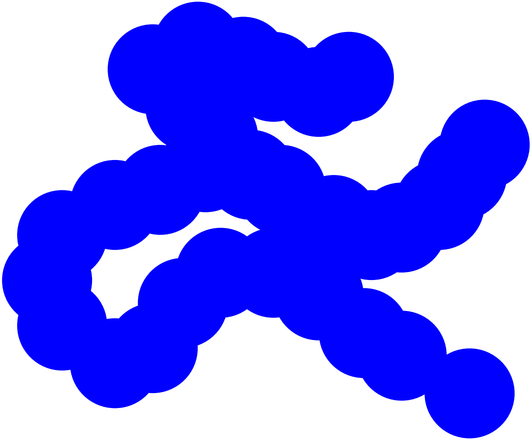

$\dim(H_0) = 1 \qquad \dim(H_1) = 1$

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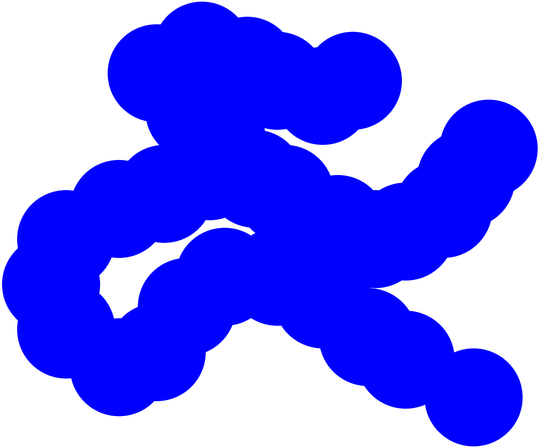

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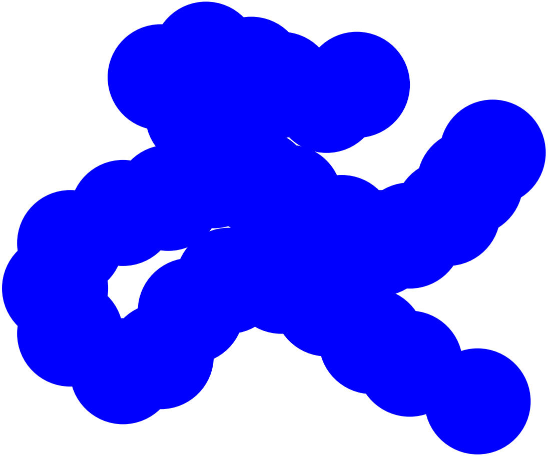
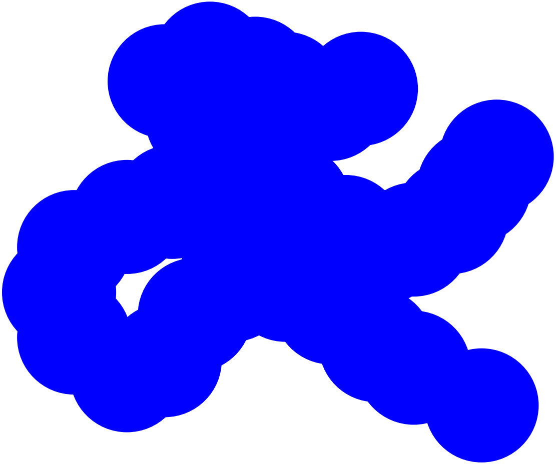


$\dim(H_0) = 1 \qquad \dim(H_1) = 3$

Example: expanding balls



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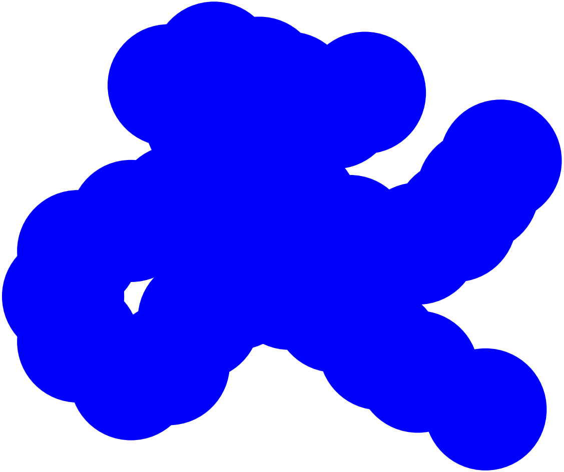

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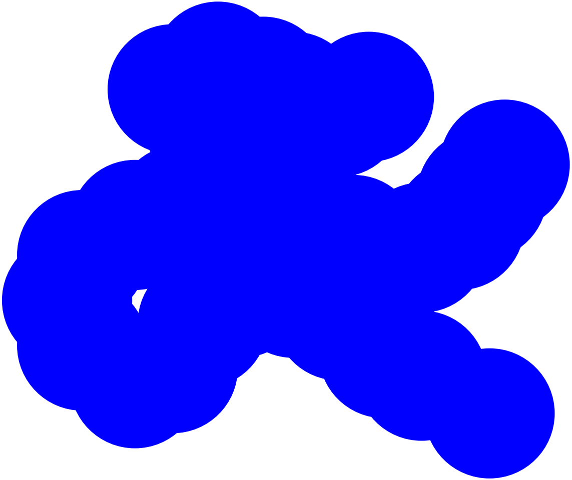

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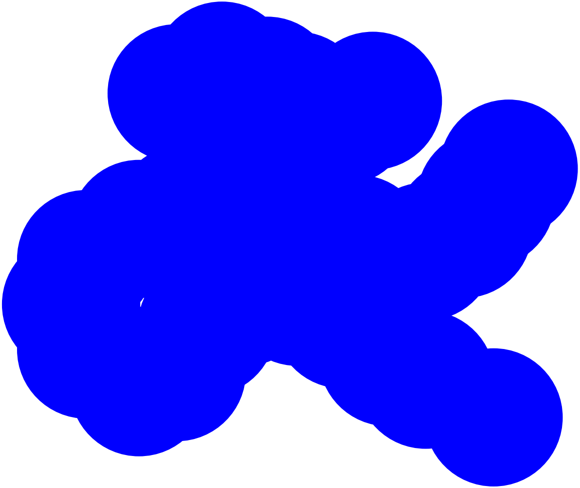

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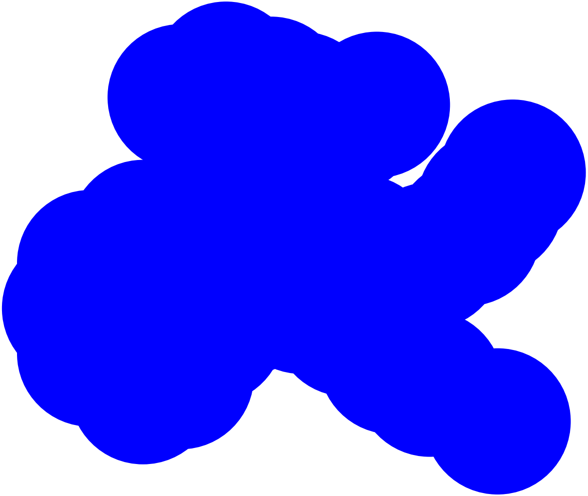

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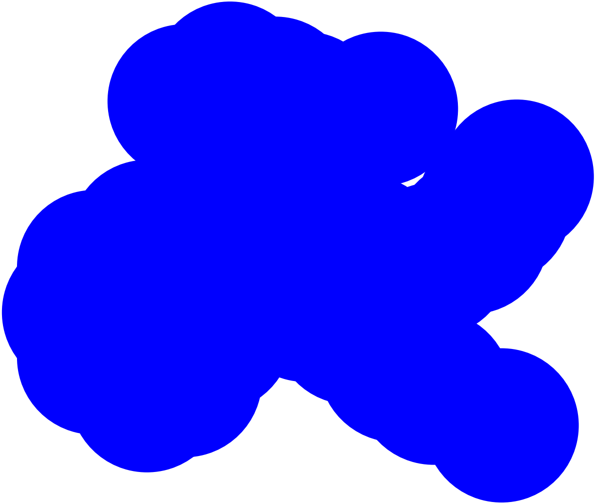

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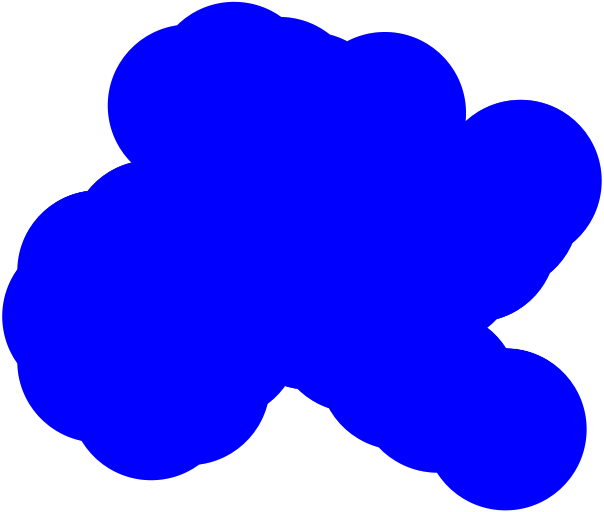

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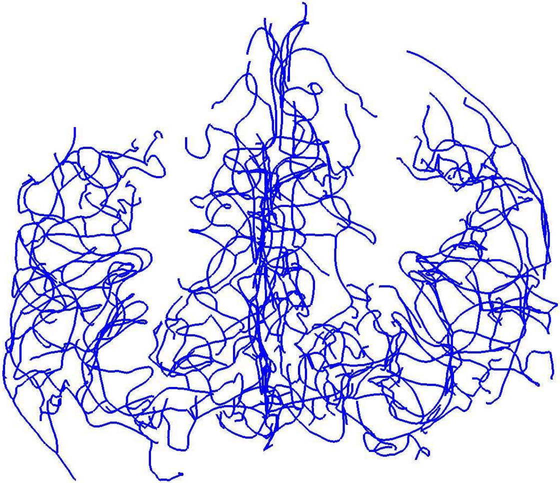
Example: filling brains [w/Bendich, Marron, Pieloch, Skwerer]



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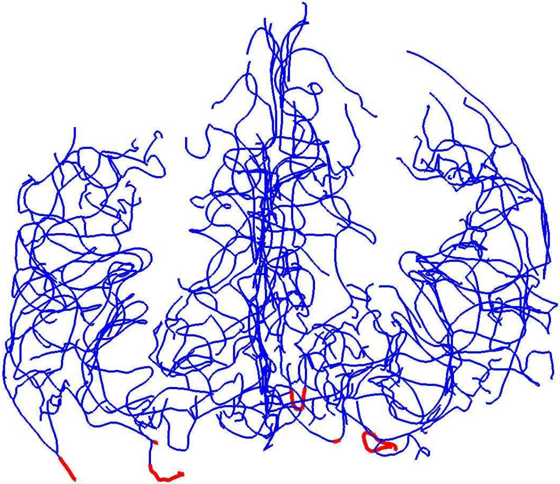

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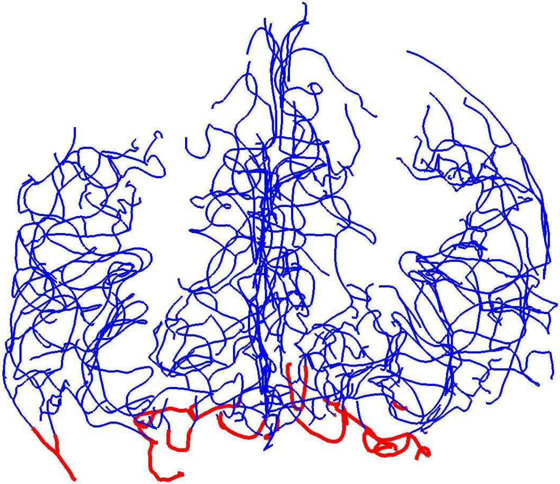

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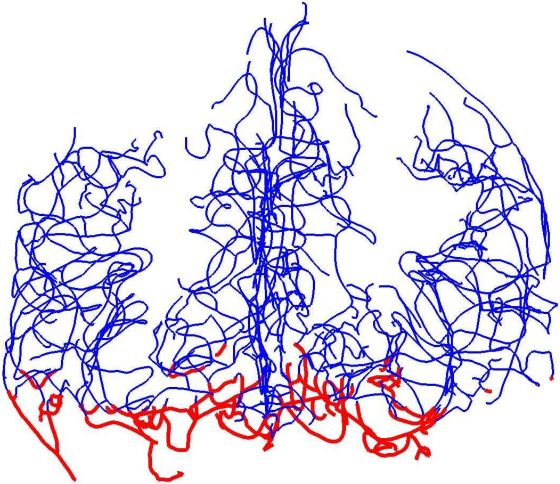

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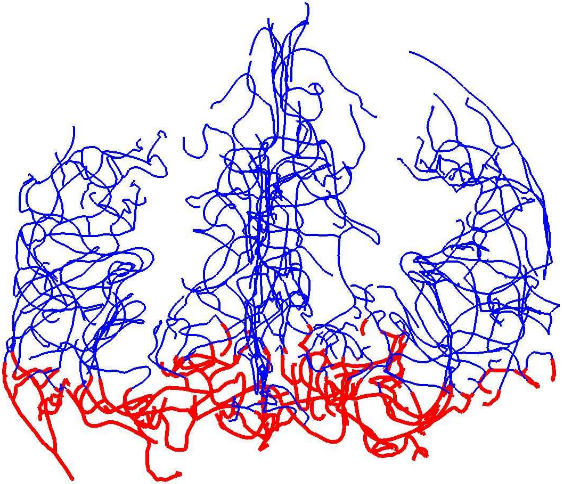

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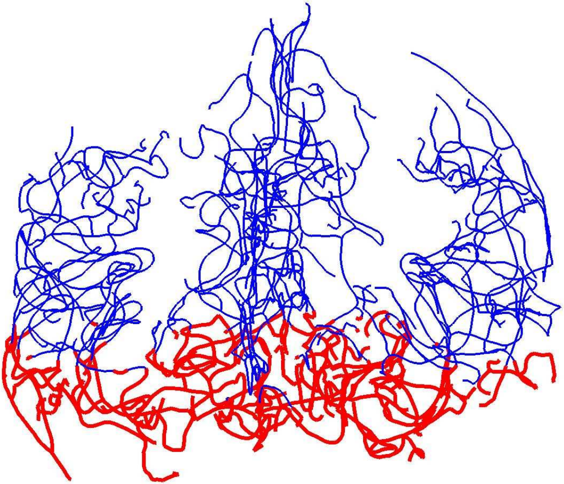

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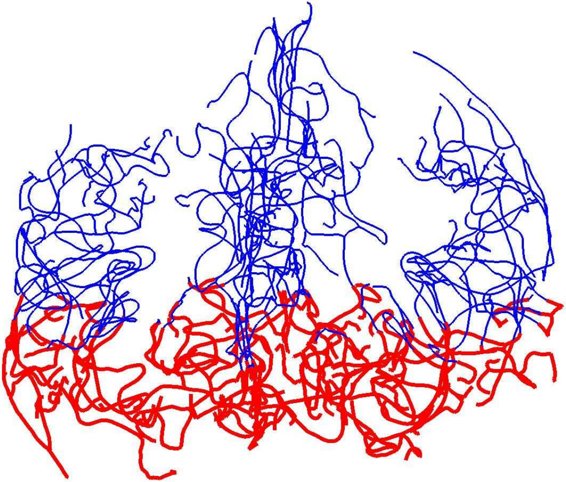

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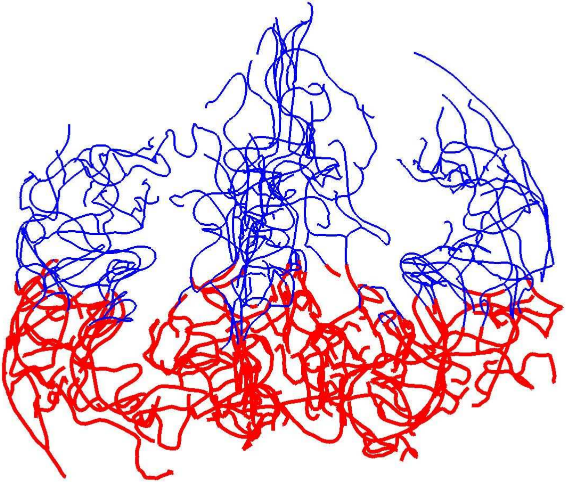

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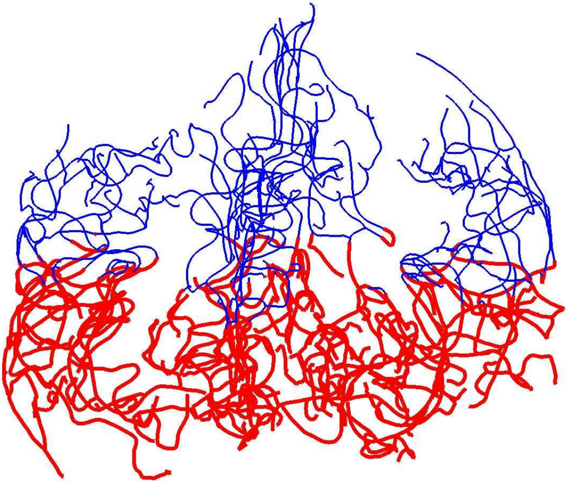

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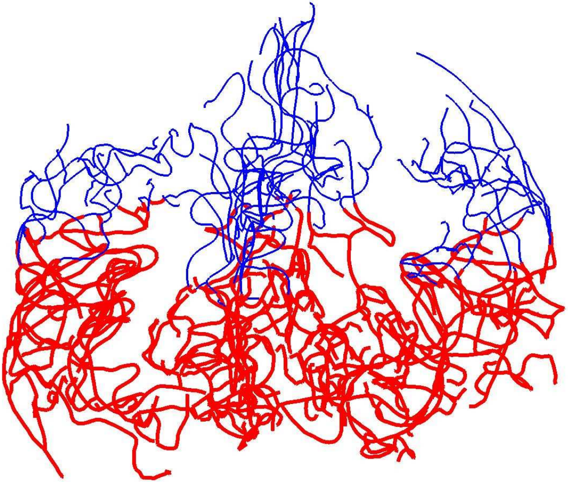

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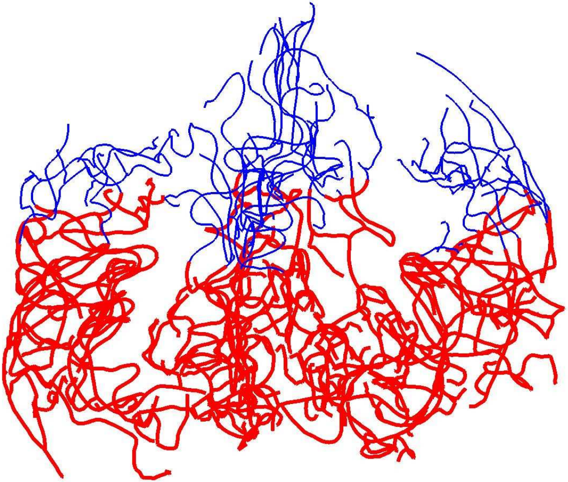

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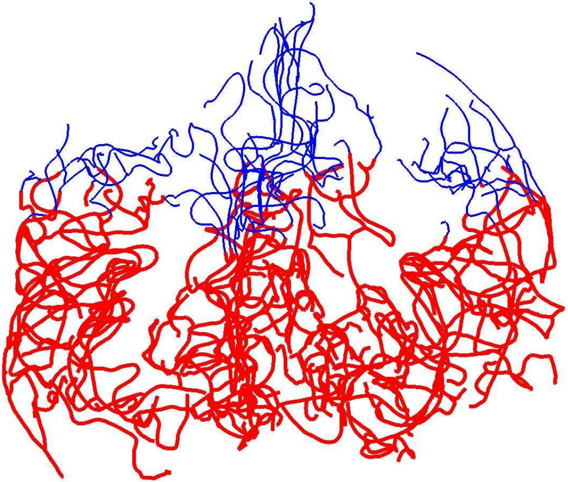

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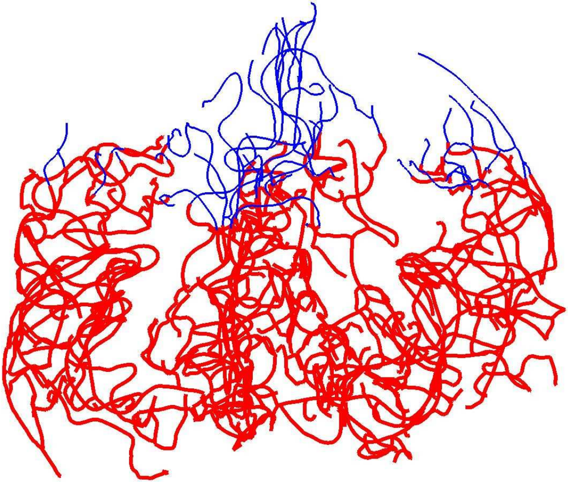

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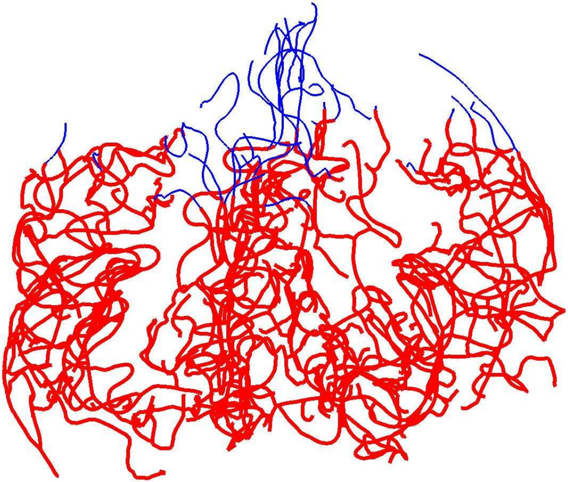

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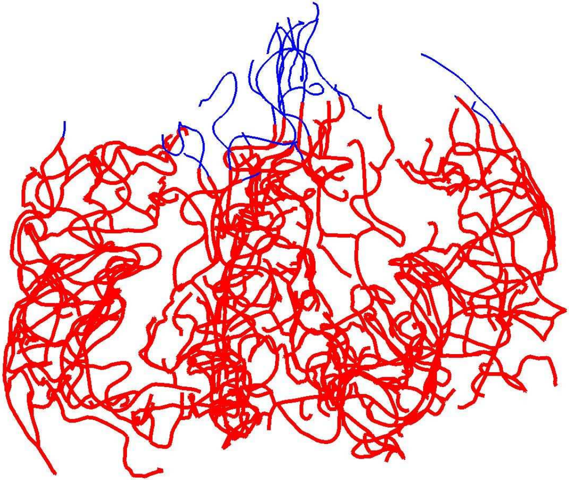

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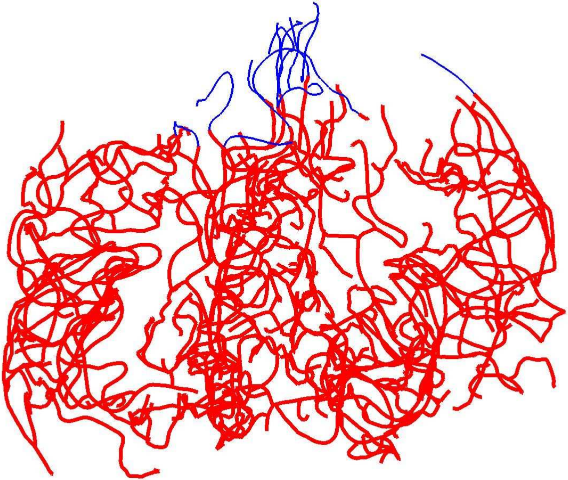

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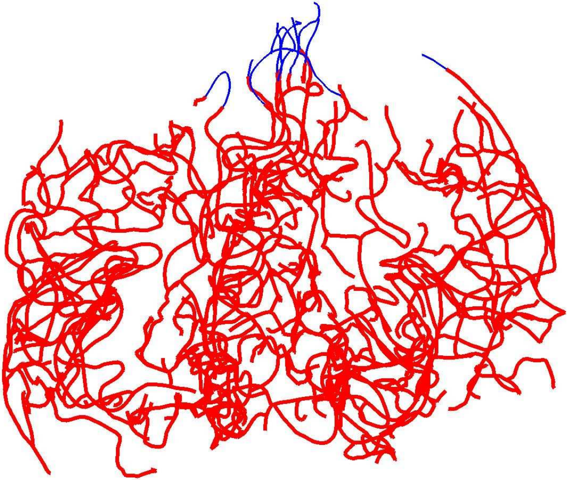

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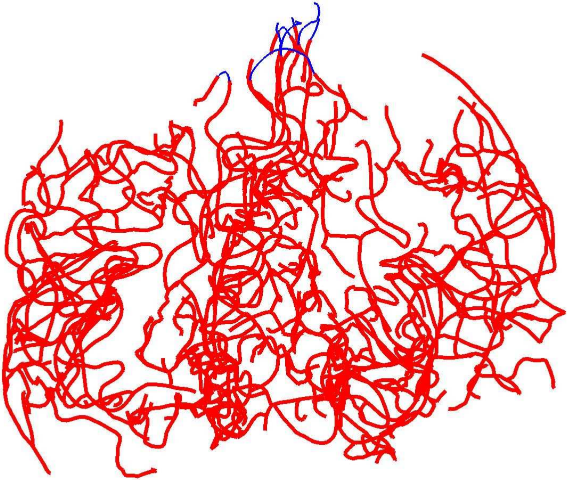

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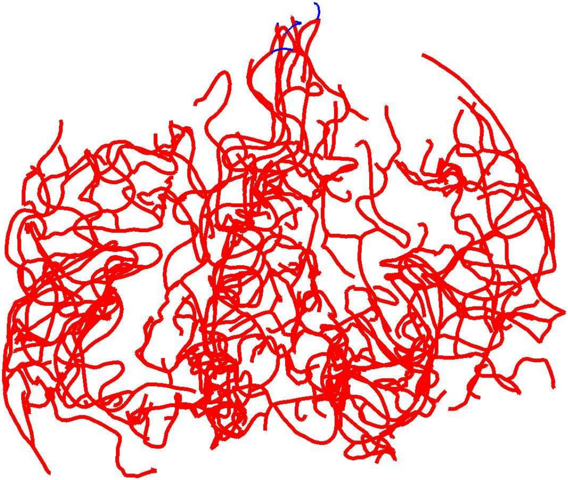

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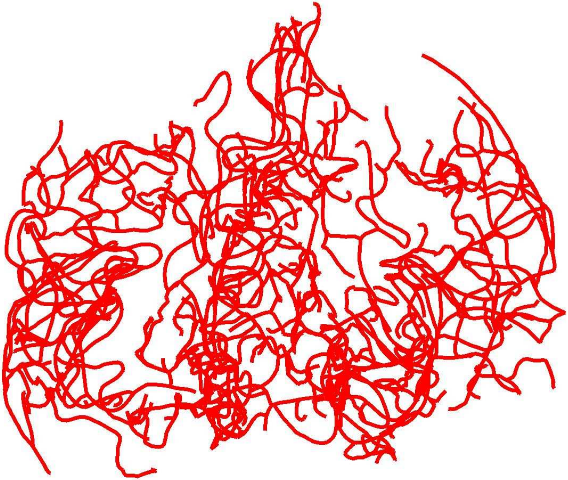

Persistent homology

Topological space X

- Fixed $X \rightsquigarrow$ homology $H_i X$ for each dimension i
- Build X step by step: measure evolving topology

Def. Let $X_\bullet$ be a filtered space, meaning $\varnothing = X_0 \subset X_1 \subset \cdots \subset X_m = X$.
The persistent homology $H_i X_\bullet$ is $H_i X_1 \to H_i X_2 \to \cdots \to H_i X_m$, a sequence of vector space homomorphisms.

Examples

1. Given a function $f : X \to \mathbb{R}$, let $X_k = f^{-1}\big((-\infty, t_k]\big)$. Choose $t_0, \ldots, t_m \in \mathbb{R}$ so $H_i X_t$ changes from t_k to t_{k+1}
2. Any simplicial complex: build it simplex by simplex in some order

History. invented by [Frosini, Landi 1999], [Robins 1999];
[Edelsbrunner, Letscher, Zomorodian 2002]: includes efficient computation;
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Multiparameter persistence

Plan. (with Houle, Curry, Thomas, +. . .) Encode 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

- models intersection homology [Bendich, Harer 2011] at undetermined scale:
- disallow interaction of larger strata with smaller ones
- diminutive features can represent new strata at appropriate scales

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

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 & {} & {} & {} & \\
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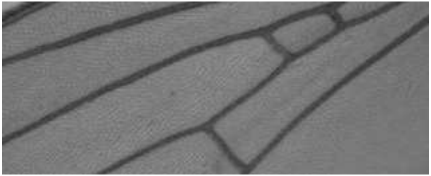

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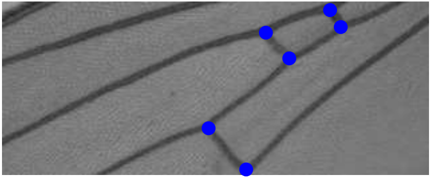

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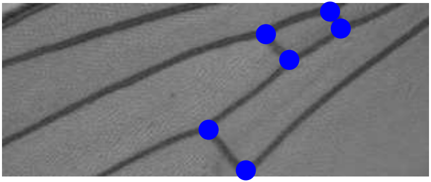

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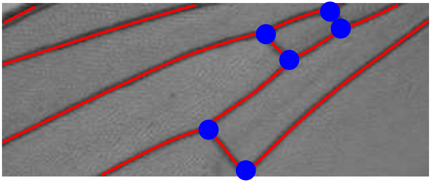

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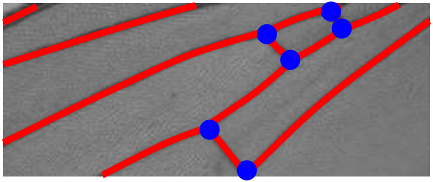

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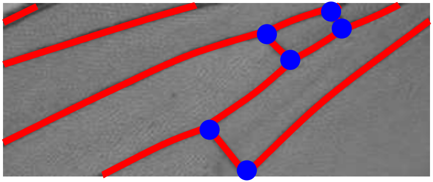

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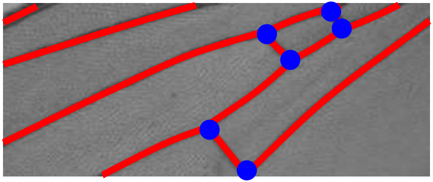

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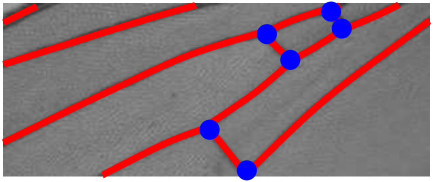

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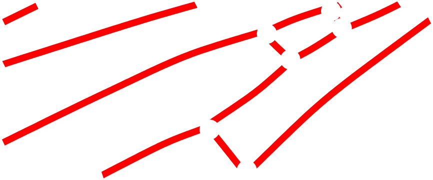

Sublevel set $W_{r,s}$ is near edges but far from vertices

- models intersection homology [Bendich, Harer 2011] at undetermined scale:
- disallow interaction of larger strata with smaller ones
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$\mathbb{Z}^2$-module:

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Plan. (with Houle, Curry, Thomas, +...) Encode with 2-parameter persistence

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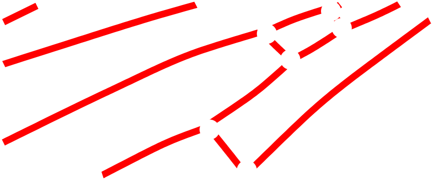

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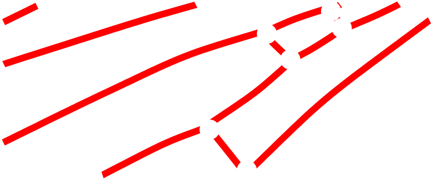

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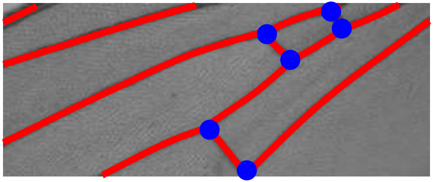

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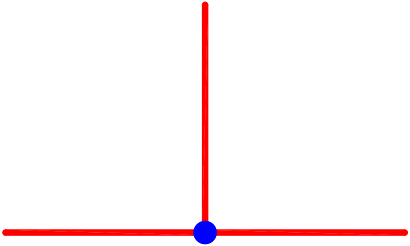
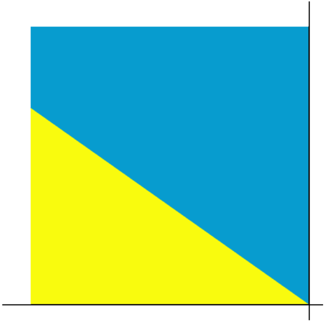


A piece of fly wing vein

$\rightsquigarrow$



The (r, s)-plane $\mathbb{R}^2$

Observations

- stratification alters persistence module
- discretization approximates something algebraic

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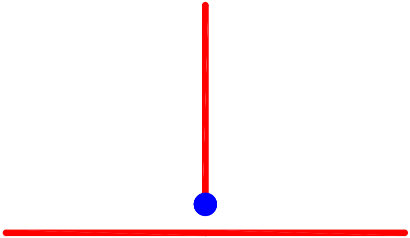

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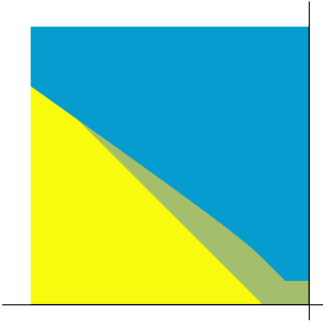

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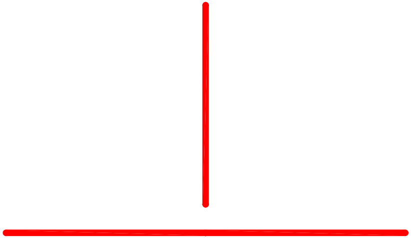

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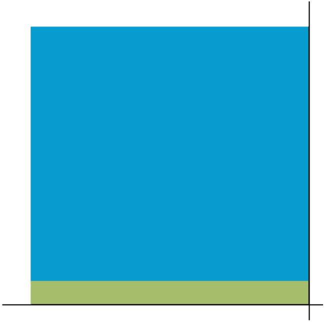

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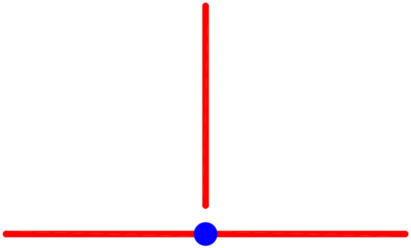

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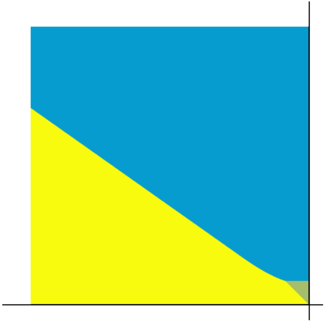

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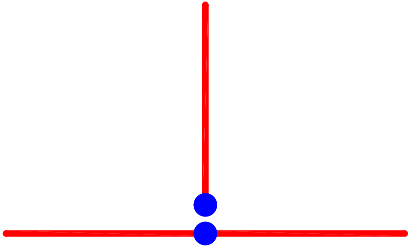

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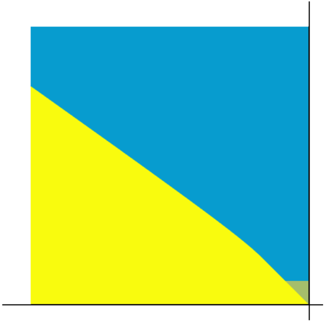

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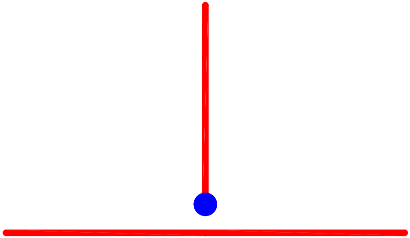

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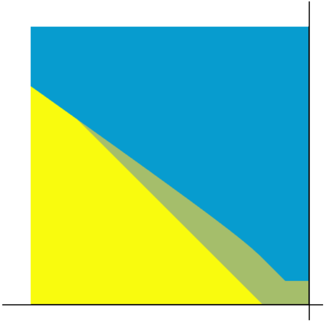

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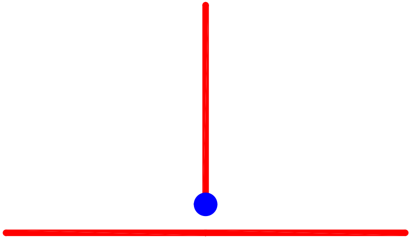

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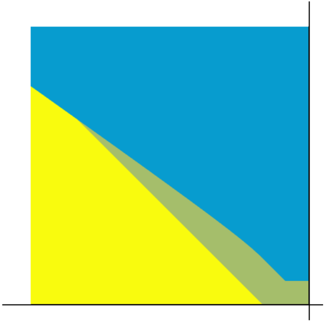

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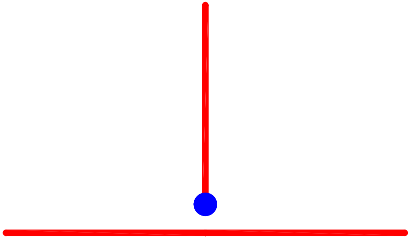

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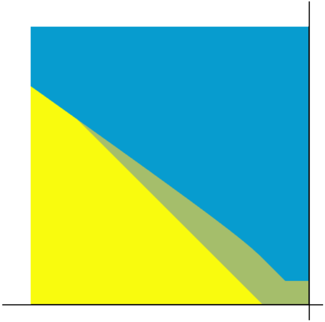

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Filter X by poset Q of subspaces: $X_q \subseteq X$ for $q \in Q \Rightarrow$ persistent homology is a

Def. Q-module:

- Q-graded vector space $H = \bigoplus_{q \in Q} H_q$ with
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Finiteness conditions: • $\mathbb{Z}^n$-modules: finitely generated $\Leftrightarrow$ noetherian
• $\mathbb{R}^n$-modules from data analysis $\leftrightarrow$??

Def. H induces isotypic regions in Q: equivalence classes for equivalence relation generated by $\mathbf{a} \sim \mathbf{b}$ whenever • $\mathbf{a} \preceq \mathbf{b}$ in Q
and • $H_\mathbf{a} \xrightarrow{\sim} H_\mathbf{b}$.

H is tame if $\dim_\Bbbk H_q < \infty$ and $\#$isotypic regions $< \infty$.

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Def [w/Curry & Thomas]. H has finite encoding $\pi : Q \to P$ if

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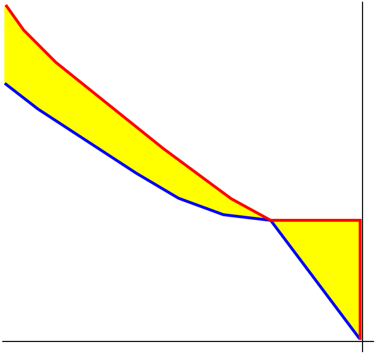
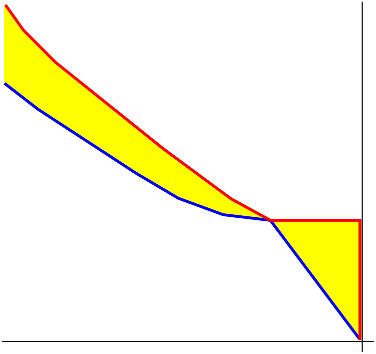


An $\mathbb{R}^2$-module

$\rightsquigarrow$



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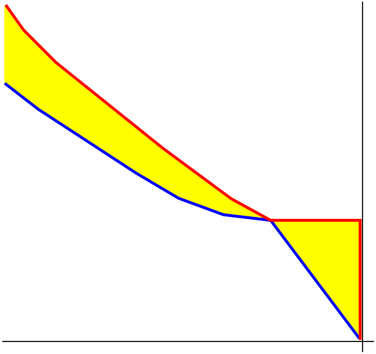

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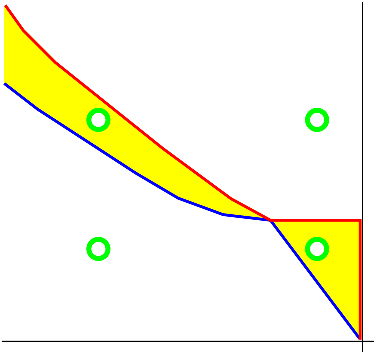

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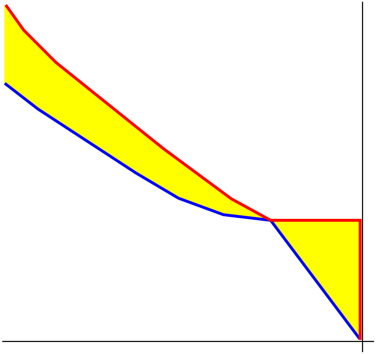

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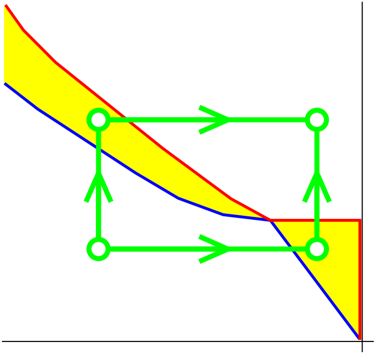

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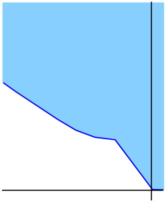
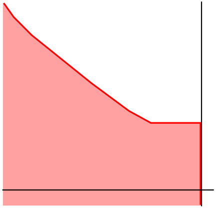
$U =$  and  $= D$

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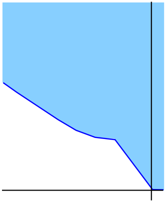

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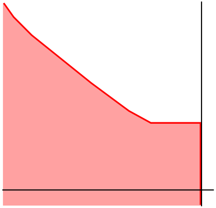

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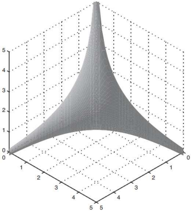
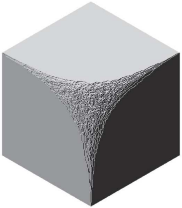


semialgebraic

or



piecewise linear

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[Andrei Okounkov, *Limit shapes, real and imagined*, Bulletin of the AMS **53** (2016), no. 2, 187–216]

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birth upsets →

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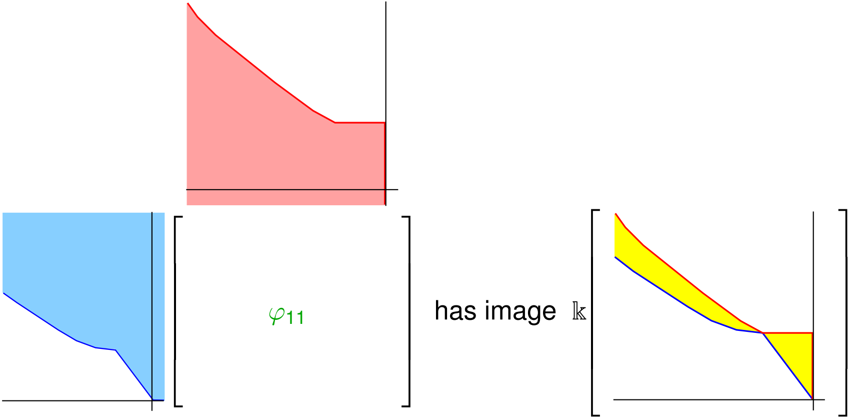

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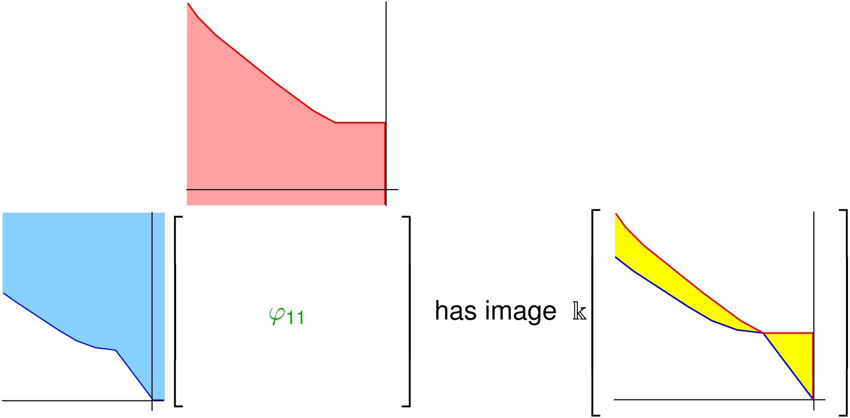

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For any subset $S \subseteq Q$, set $\mathbb{k}[S] = \bigoplus_{s \in S} \mathbb{k}_s$.

Def [w/Curry & Thomas]. A fringe presentation of H is a monomial matrix

← death downsets

birth upsets →

← scalar entries

$$\mathbb{k}[U_1] \oplus \cdots \oplus \mathbb{k}[U_k] = F \xrightarrow{\begin{array}{cc} & \begin{array}{ccc} D_1 & \cdots & D_\ell \end{array} \\ \begin{array}{c} U_1 \\ \vdots \\ U_k \end{array} & \begin{bmatrix} \varphi_{11} & \cdots & \varphi_{1\ell} \\ \vdots & \ddots & \vdots \\ \varphi_{k1} & \cdots & \varphi_{k\ell} \end{bmatrix} \end{array}} E = \mathbb{k}[D_1] \oplus \cdots \oplus \mathbb{k}[D_\ell]$$

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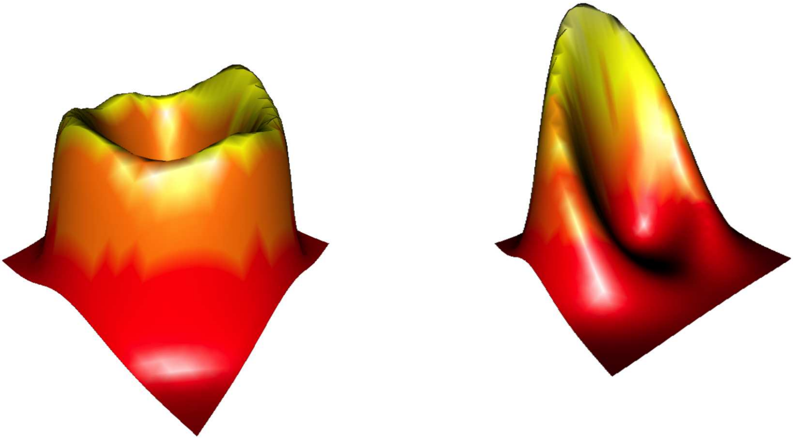

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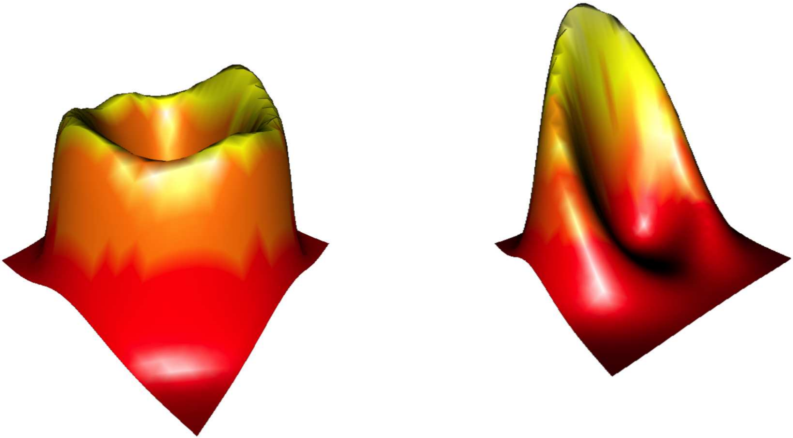

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Future directions

Algebra

- QR codes: (co)generator functors and primary decomp. of $\mathbb{R}^n$-modules
- Syzygy conj: $\mathbb{R}^n$-modules have indicator-homological dimension $\leq n$

Geometric statistics

- geometric probability/statistics on stratified spaces
- No-moduli conj: rank function $\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{N}$ determines H_0 and H_{n-1} modules for objects in $\mathbb{R}^n$ $(\mathbf{a} \preceq \mathbf{b}) \mapsto \operatorname{rank}(H_\mathbf{a} \to H_\mathbf{b})$
- Local statistical sufficiency conj: Different fly wings yield nonisomorphic modules locally; i.e., deformation of fly wing splines ⇒ QR code changes

Computation

- calculate encoding / fringe presentation from vertices and Bézier curves
- homological algebra with semialgebraic indicator modules
- data structures for rank functions; computation for statistics

Topology. Biparameter persistence as persistent intersection homology

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- calculate encoding / fringe presentation from vertices and Bézier curves
- homological algebra with semialgebraic indicator modules
- data structures for rank functions; computation for statistics

Topology. Biparameter persistence as persistent intersection homology

Biology. The topological novelty hypothesis

Future directions

Algebra

- QR codes: (co)generator functors and primary decomp. of $\mathbb{R}^n$-modules
- Syzygy conj: $\mathbb{R}^n$-modules have indicator-homological dimension $\leq n$

Geometric statistics

- geometric probability/statistics on stratified spaces
- No-moduli conj: rank function $\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{N}$ determines H_0 and H_{n-1} modules for objects in $\mathbb{R}^n$ $(\mathbf{a} \preceq \mathbf{b}) \mapsto \operatorname{rank}(H_{\mathbf{a}} \to H_{\mathbf{b}})$
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Thank You