Computing homology robustly: from persistence to the geometry of normed chain complexes

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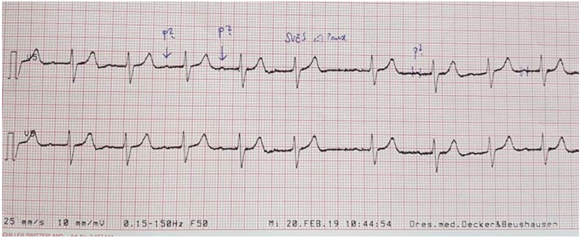
Examining images of porous rock to decide whether it is permeable or not is a question of topology.

In an electrocardiogram, what counts are the peaks (number, approximate height), not their exact temporal location. It's the landscape after reparameterization, i.e. above all topological information.



Multidimensional version: density-guided classification (F. Chazal, L. Guibas, S. Oudot, P. Skrabas)

Datum: a finite metric space.

First step. A local density is calculated. The algorithm first divides the space into clusters, which are the basins of attraction of the gradient of the density. There are too many of them: as many as there are local maxima.

Second step. The algorithm merges the clusters corresponding to maxima that are not sufficiently accentuated.

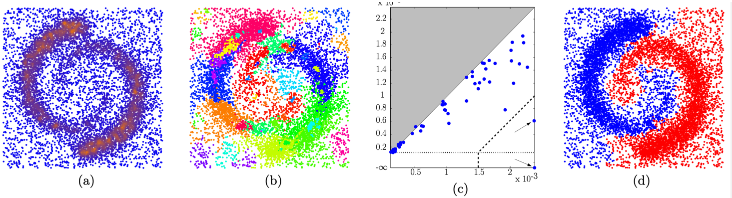


Figure 2: Our approach in a nutshell: (a) estimation of the underlying density function f at the data points; (b) result of the basic graph-based hill-climbing step; (c) approximate PD showing 2 points far off the diagonal corresponding to the 2 prominent peaks of f; (d) final result obtained after merging the clusters of non-prominent peaks.

The method gave excellent results on cytology data (cell classification based on photos).

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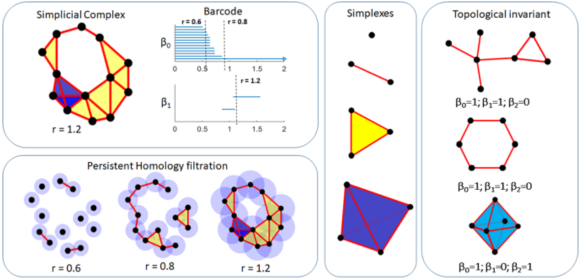
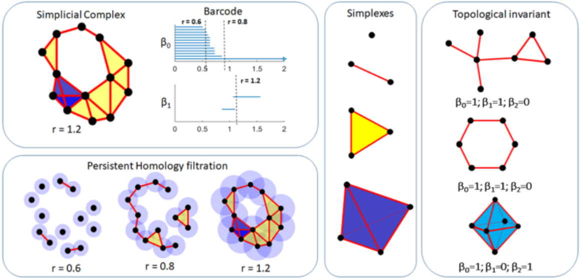
It is associated with a growing family of simplicial polyhedra: N_r is the nerve of the covering by balls of radius r.





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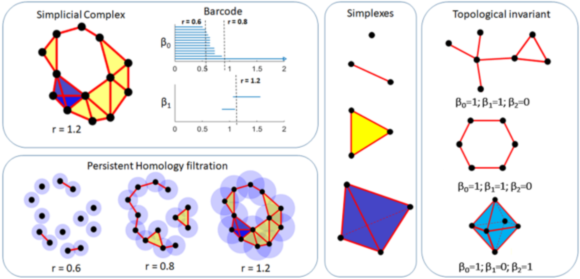
We calculate the homology with coefficients in $\mathbb{F}_2$, $H_k(N_r, \mathbb{F}_2)$, for each r.



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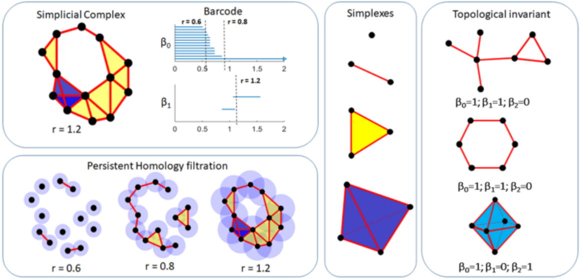
Disadvantage. $H_k(N_r, \mathbb{F}_2)$ is very unstable.

How do you extract stable information?



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We can detect when a homology class is born (it does not belong to $im(H_k(N_{r-\epsilon}, \mathbb{F}_2) \to H_k(N_r, \mathbb{F}_2))\ \forall\epsilon$) and when it dies, hence a collection of intervals $[r, s]$, the *barcode*.

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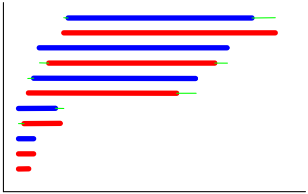
The *bottleneck distance* between two barcodes is obtained by matching the bars as closely as possible, even if this means discarding bars that are too short.



Theorem (Stability: Cohen-Steiner, Edelsbrunner, Harer 2005)

$$\textit{bottleneck dist.(barcodes)} \leq \textit{Hausdorff dist.(point clouds)}.$$

The stability theorem invites us to neglect the small bars. What does what remains mean?

Theorem (Meaning of large bars: Chazal, Lieutier 2005)

If a subset $X \subset \mathbb{R}^N$ has Weak feature size 4ϵ, and if

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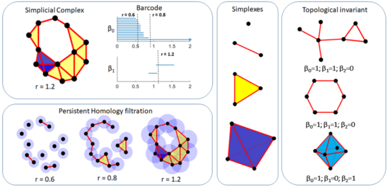
Moral: given a somewhat regular object, we can calculate its topology (at least, its homology) from a fairly dense sample, with theoretical guarantees.

The homology of simplicial complexes is linear algebra. Consider the vector space (on $\mathbb{F}_2$ or $\mathbb{R}$) whose base is the set of simplices (vertices, edges, faces, etc.). Here, of dimension 48 (13 vertices, 23 edges, 11 faces, 1 tetrahedron).



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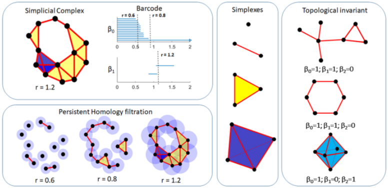

The boundary of a simplex is a linear combination of other simplices, hence a linear map ∂, and its adjoint d. The boundary of the boundary is zero: $\partial \circ \partial = 0$, hence $d \circ d = 0$. In particular, $\mathrm{Im}(\partial) \subset \mathrm{Ker}(\partial)$, $\mathrm{Im}(d) \subset \mathrm{Ker}(d)$. We define

$$\text{homology} \ = \mathrm{Ker}(\partial)/\mathrm{Im}(\partial), \quad \text{cohomology} \ = \mathrm{Ker}(d)/\mathrm{Im}(d).$$

Both count holes, i.e. cycles that are not boundaries.

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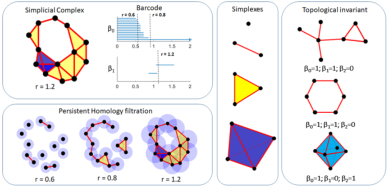

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More generally, a *chain complex* is a vector space B provided with a linear map d such that $d \circ d = 0$.

Question. What are the robustness guarantees for calculating the homology of a chain complex?

We've seen how persistent homology provides robustness. In numerical analysis, robustness is achieved by another means.

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If we change b to $b' = b + \Delta b$, the solution changes to $x' = x + \Delta x$, such that

$$\frac{|\Delta x|}{|x|} \leq \kappa(F)\frac{|\Delta b|}{|b|}.$$

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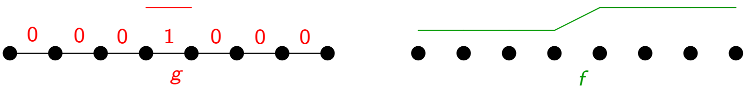
When $d : B \to B$ is a chain complex (i.e. $d \circ d = 0$), we're interested in the conditioning number of $\bar{d} : B/\mathrm{Ker}(d) \to \mathrm{Im}(d)$. In infinite dimension, it can be infinite.

We equip the cochains of a simplicial complex with ℓ^p norms.

Example. The n-stick satisfies $H^1 = 0$. The 1-cochain g equal to $\bar{1}$ on the central edge and 0 elsewhere can be written df where

$$\|g\|_p = 1, \quad \|f\|_p \sim n^{1/p}.$$



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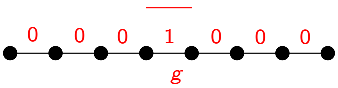

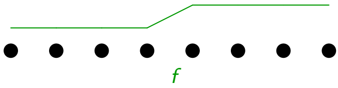

When n is large, solving $df = g$ is unstable. The homology calculation is ill-conditioned.

Definition

The **conditioning number** *of a graph X is $\kappa(X, p, \mathbf{k}) = |\bar{d}||\bar{d}^{-1}|$ where $\bar{d} : C(X, \mathbf{k})/\mathrm{Ker}(d) \to dC(X, \mathbf{k})$. (It depends on p and the field $\mathbf{k}$).*

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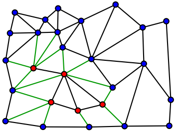
$|A| = 5$, $|\partial A| = 15$.



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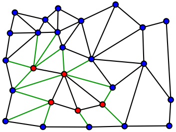

Definition

Cheeger's constant $h(X)$ *of a graph* X *is the largest* h *such that for every set* A *of vertices such that* $|A| \leq \frac{1}{2}|X|$,

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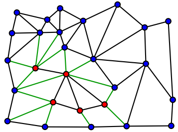

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Proposition

$$h(X) = \frac{2}{\kappa(X,1,\mathbb{F}_2)} = 2(\|\bar{d}\|_{1\to 1}\|\bar{d}^{-1}\|_{1\to 1})^{-1} \text{ over } \mathbb{F}_2.$$

Proposition

Let Δ be the self-adjoint operator corresponding to the quadratic form $f \mapsto \|df\|_2^2 = \langle f, \Delta f\rangle$. Let $\lambda_1 \leq \lambda_2 \leq \cdots$ denote its eigenvalues. If the graph X is connected, then $\lambda_1 = 0$ and

$$\lambda_2 = (\|\bar{d}^{-1}\|_{2\to 2})^{-2}.$$

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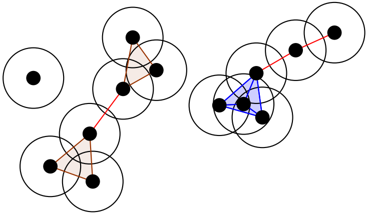
Moral: normed chain complexes contain interesting information, beyond their mere homology.

Given a metric space X, a finite subset $Y \subset X$ and $r > 0$, the *Čech simplicial complex* Y_r has a simplex $(y_0, \ldots, y_k)$ each time $\bigcap_i B(y_i, r) \neq \emptyset$. Let $C_\cdot^r$ denote the simplicial chains of Y_r.



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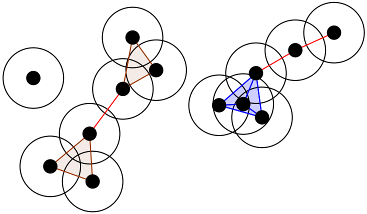

Theorem (Bobrowski-Weinberger 2017)

Fix $r < \frac{1}{2}$ and $1 \leq k \leq d$. Let Y be an n-sample picked at random on the standard d-torus. Then, with high probability, the k-homology of Y_r coincides with the homology of the torus as soon as

$$\omega_d r^d \, n \gg \log n + k \log \log n,$$

and this fails if $\omega_d r^d \, n \ll \log n + (k-2) \log \log n$. If $k = 0$, the threshold is $2^{-d} \log n$.

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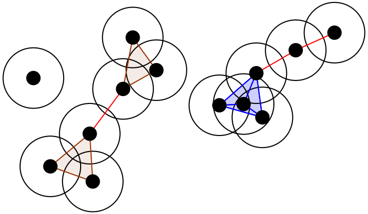

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Question. Can one say that the chain complexes $C_\cdot^r$ converge to some chain complex attached to the torus?

In order to define a distance between normed chain complexes, the first idea is to measure conditioning numbers of isomorphisms.

Definition

Let $B_1 \overset{d_1}{\to} B_1$ *and* $B_2 \overset{d_2}{\to} B_2$ *be normed chain complexes. The* **Banach-Mazur distance** $\mathrm{BMDist}(B_1, B_2)$ *is the infimum of* $\log(|F||F^{-1}|)$ *over all isomorphisms* $F : B_1 \to B_2$ *duch that* $Fd_1 = d_2F$*.*

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This is too restrictive: this implies $\dim(B_1) = \dim(B_2)$.

The second idea is too measure the size of homotopies.

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Let $B_1 \stackrel{d_1}{\to} B_1$ *and* $B_2 \stackrel{d_2}{\to} B_2$ *be normed chain complexes. Consider all bounded homotopies, i.e.*

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$$1 - F_2 F_1 = d_1 Q_1 + Q_1 d_1, \quad 1 - F_1 F_2 = d_2 Q_2 + Q_2 d_2.$$

Let $q = \max\{|Q_1|, |Q_2|\}$, $f = \max\{1, |F_1||F_2|\}$. *The* **homotopy distance** $\mathrm{HomDist}(B_1, B_2)$ *is the infimum over all homotopies of* $\min\{\frac{q}{f} + \log f, \frac{f}{q} + \log q\}$.

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The weird expression guarantees a triangle inequality.

Definition

Let Null denote the set of null normed chain complexes (i.e. with $d = 0$). Denote by

$$\mathrm{ND}(B) = \mathrm{HomDist}(B, \mathit{Null}), \quad \mathrm{NH}(B) = |\bar{d}^{-1}|.$$

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$$\sigma_j = \inf\{s \geq 0\,;\, \exists L \subset \bar{B} \text{ subvectorspace such that } \dim(L) \geq j \text{ and } \forall \bar{x} \in L,\ |\bar{d}\bar{x}| \leq s|\bar{x}|\}.$$

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Fact. Each σ_j is continuous in homotopy distance.

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Fact. A prehilbertian chain complex is precompact $\iff$ its singular values form a sequence that tends to $+\infty$.

Proposition

Let B_i be precompact prehilbertian chain complexes. Then B_i converges to B $\iff$ for every j, $\sigma_j(B_i)$ tends to $\sigma_j(B)$.

Analogy between normed chain complexes and metric spaces.

Metric space	Normed chain complex
Gromov-Hausdorff distance	Homotopy distance
Point	?
Bounded	?
Precompact	?
Compactness criterion (Gromov)	?

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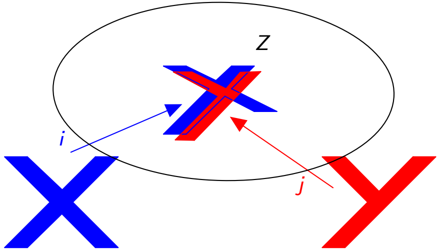
Let X, Y be metric spaces.

$$GHDist(X,Y) = \inf\{HDist_Z(i(X), j(Y))\,;\, Z \text{ metric space},\\ i : X \to Z,\, j : Y \to Z \text{ isometric embeddings}\}.$$



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B is homotopic to a null complex $\iff \mathrm{ND}(B) < \infty$.

One can think of $\mathrm{ND}(B) = \mathrm{HomDist}(B, Null)$ as an analogue of diameter.

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B is precompact $\implies$ the singular values of B form a sequence that tends to $+\infty$ ($\iff$ if B is prehilbertian).

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Definition

X precompact metric space, $\epsilon > 0$. The **covering number** $N(X, \epsilon)$ *is the minimal number of ϵ-balls that can cover X.*

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Theorem (Gromov's compactness criterion)

A collection $\mathcal{T}$ of precompact metric spaces is precompact in Gromov-Hausdorff distance if and only if there is a function ν which serves as a covering number for all spaces in $\mathcal{T}$, i.e.

$$\forall \epsilon > 0, \quad \forall X \in \mathcal{T}, \quad N(X, \epsilon) \leq \nu(\epsilon).$$

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Compactness criterion (Gromov)	Common profile

Definition

Let (B, d) be a normed chain complex that belongs to the closure of finite dimensional normed complexes. Its **profile** *is the "smallest" function $\pi = (\pi_d, \pi_c) : (0, +\infty) \to (0, +\infty)^2$ with the following property. For every $\epsilon > 0$, there exists a finite-dimensional normed complex (B', d') such that*

$$HomDist(B, B') < \epsilon, \quad \dim(B') \leq \pi_d(\epsilon), \quad \kappa(B', d') \leq \pi_c(\epsilon).$$

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Theorem

A collection of nonnull normed chain complexes is precompact if and only if a same profile serves for all and the distances to null complexes are bounded below.

Lemma

Let B be a prehilbertian chain complex. Then the profile of B is determined by the asymptotics of eigenvalues,

$$\pi_d(\epsilon) \leq \mathrm{Card}\{\lambda \in \mathrm{spectrum}(d^* d)\,;\ \lambda < \frac{1}{\epsilon^2}\}, \quad \pi_c(\epsilon) \leq \frac{1}{\epsilon\sqrt{\lambda_2}}.$$

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Example

Let M be a smooth compact Riemannian manifold. Consider the (de Rham) complex of smooth differential forms on M in its L^2 norm. Its profile satisfies $\pi_d(\epsilon) \leq C\,\epsilon^{-N}$, where $N = \dim(M)$.

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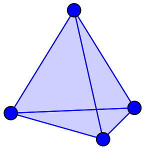
Let Y be a finite metric space. The *complete simplicial complex* Δ_Y on Y takes as simplices all tuples of points of Y. Pick a function of the diameter as a weight,

$$w(\sigma) = \phi(\mathrm{diam}(\sigma)).$$

Use weighted ℓ^p norms on cochains. This gives a normed chain complex $C^{\cdot}(Y)$.



The complete simplicial complex on 4 points.

Let (X, μ) be a metric measure space. Same construction with the same weight w and $L^p(\mu^{\otimes \cdot})$ norms yields a normed chain complex $C^\cdot(X, \mu)$.

Example. 1-cochains are functions c on $X \times X$. The squared weighted L^2 norm is

$$\int_{X \times X} \phi(|x - x'|)|c(x, x')|^2 \, d\mu(x) \, d\mu(x').$$

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Theorem (Burago-Ivanov-Kurylev 2015)

Take $\phi = 1_{[0,\rho]}$. Stick to spaces where the measures of balls vary continuously in a quantitative manner. Laplace eigenvalues below $2\rho^{-2}$ are continuous functions of (X,μ) in L^∞ Gromov-Wasserstein distance (a topology that combines Gromov-Hausdorff and weak measure convergence).

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Question. Study steeper weights, like $\phi(\delta) = 1_{[0,\rho]} \frac{1}{\delta^k}$ in degree k. Do Laplace eigenvalues on $C^k(X, \mu)$ depend continuously on (X, μ)?

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If G is an infinite graph, the chain complex $\ell^p C^{\cdot}(G)$ is not precompact.

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Example

The chain complex $\ell^p C^\cdot(\mathbb{Z} \star \mathbb{Z})$ has finite nulldistance for all $p \geq 1$.

So it is the analogue of a bounded noncompact metric space.

Question. What is the analogue of pointed Hausdorff convergence?