

Computational Homology Project (CHomP)

<http://chomp.rutgers.edu/>

Konstantin Mischaikow

Mathematics and BioMaPS Institute
Rutgers University

mischaik@math.rutgers.edu

Computing Homology

1. Homology
2. Geometric Complexes
3. Geometric Preprocessors
4. Maps

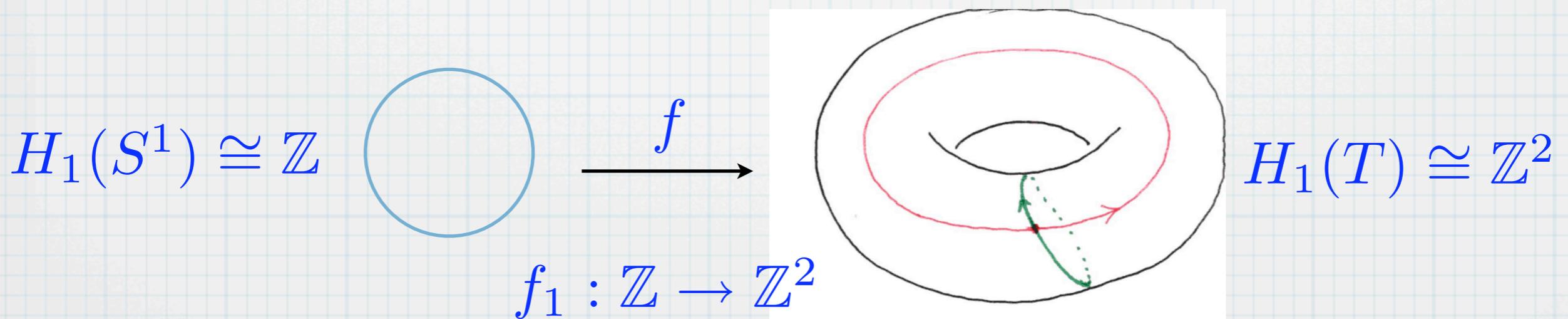
1. Homology

X a topological space $\Rightarrow H_*(X)$ an ~~abelian group~~ ^{vector space}

$$H_k(X, \mathbb{Z}_2) \cong \mathbb{Z}_2^{\beta_k}$$

Betti number

$f : X \rightarrow Y$ continuous map $\Rightarrow f_* : H_*(X) \rightarrow H_*(Y)$
~~group homomorphism~~
linear map



With an appropriate choice of basis $f_1 = [a, b]$

Computing Homology

A **free chain complex** $\mathcal{C} = \{C_k, \partial_k\}_{k \in \mathbb{Z}}$ consists of free abelian groups C_k , called **chains**, and homomorphisms $\partial_k : C_k \rightarrow C_{k-1}$, called **boundary operators**, such that

$$\partial_k \circ \partial_{k+1} = 0.$$

The **cycles** are the subgroups $Z_k := \ker \partial_k$.

The **boundaries** are the subgroups $B_k := \text{image } \partial_{k+1}$.

The **k -th Homology group** is

$$H_k(\mathcal{C}) := \frac{Z_k}{B_k}$$

Theorem: (Smith Normal Form) Given a matrix $A : \mathbb{Z}^n \rightarrow \mathbb{Z}^m$ there exist invertible matrices $R : \mathbb{Z}^n \rightarrow \mathbb{Z}^n$ and $Q : \mathbb{Z}^m \rightarrow \mathbb{Z}^m$ such that

$$B := Q^{-1}AR = \left[\begin{array}{ccc|ccc} b_1 & & & & & \\ & b_2 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & 0 & & & \cdot & \\ & & & & & b_t \\ \hline & & & & & \\ & & & 0 & & \\ & & & & & 0 \end{array} \right],$$

where b_i are positive integers, $b_i = 1$ for $i = 1, 2, \dots, s$, and b_i divides b_{i+1} for $i = 1, 2, \dots, t - 1$.

simplicial

Let $X \subset \mathbb{R}^d$ be a ~~cubical~~ set. The boundary map $\partial_k : C_k(X) \rightarrow C_{k-1}(X)$ takes the form of a matrix

$$A_k : \mathbb{Z}^{d_k} \rightarrow \mathbb{Z}^{d_{k-1}}$$

simplicies

where the basis is defined by the ~~elementary cubes~~.

$$\begin{array}{ccccc}
 & & \mathbb{Z}^{d_k} & \xrightarrow{B_k} & \mathbb{Z}^{d_{k-1}} \\
 & & \uparrow R_k & & \downarrow Q_{k-1}^{-1} \\
 C_{k+1} & \xrightarrow{\partial_{k+1}} & C_k & \xrightarrow{\partial_k} & C_{k-1} \\
 \downarrow R_{k+1} & & \uparrow Q_k^{-1} & & \\
 \mathbb{Z}^{d_{k+1}} & \xrightarrow{B_{k+1}} & \mathbb{Z}^{d_k} & &
 \end{array}$$

$$H_k(X) \cong \frac{\ker B_k}{R_k Q_k^{-1} B_{k+1}(\mathbb{Z}^{d_{k+1}})}$$

2. Geometric Complexes

Rayleigh–Benard Convection



Raw intensity image captured using 12-bit digital camera and filtering



Binary image obtained by thresholding at the median value of intensity

Data is in not in the form of a chain complex

Data sets are large

Cubical complexes

An *elementary interval* is a closed interval $I \subset \mathbb{R}$ of the form

$$I = [l, l + 1] \quad \text{or} \quad I = [l, l]$$

for some $l \in \mathbb{Z}$.

An *elementary cube* is a finite product of elementary intervals

$$Q = I_1 \times I_2 \times \cdots \times I_d \subset \mathbb{R}^d,$$

where each I_i is an elementary interval.

$$\mathcal{K}_k^d := \{k\text{-dimensional cubes in } \mathbb{R}^d\}$$

A *cubical set* is a finite union of elementary cubes

3. Geometric Preprocessors

Co-Reduction, M. Mrozek, B. Batko,

Dis. Comp. Geom. '09

Idea: Reduce the geometric complex as much as possible before building the chain complex and computing Smith Normal Form.

Fact: If $A \subset X$ is acyclic, then

$$H_k(X) \cong \begin{cases} H_k(X, A) \oplus \mathbb{Z} & \text{if } k = 0 \\ H_k(X, A) & \text{otherwise} \end{cases}$$

$$C_*(X, A) := \frac{C_*(X)}{C_*(A)}$$

Goal: Remove a “maximal” acyclic subset A of X .

The Co-Reduce Algorithm

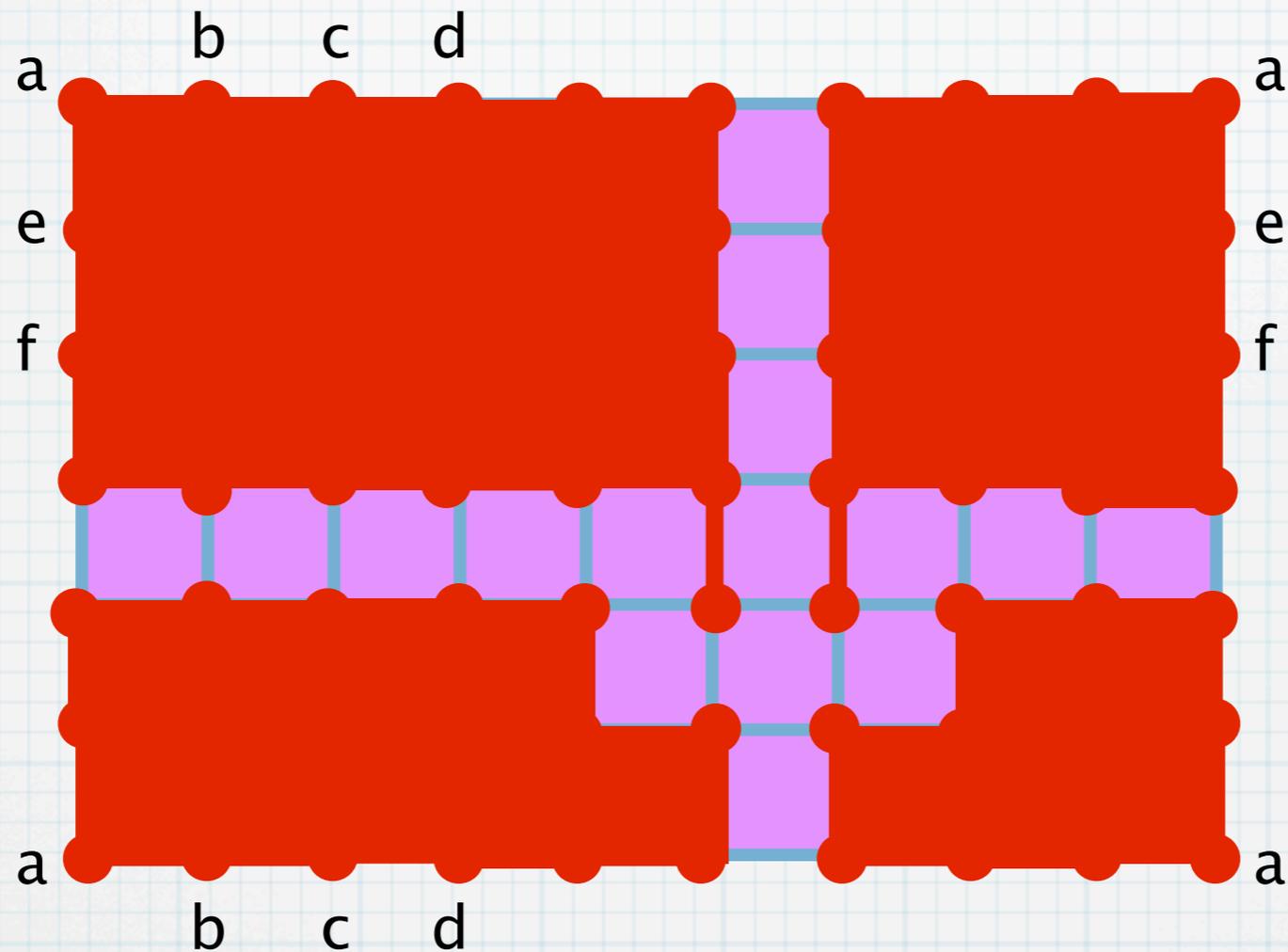
Geometric
boundary

Geometric
co-boundary

01	Queue $Q := \text{NULL}$
02	$Q \leftarrow \sigma_0$
03	while ($ Q \neq 0$)
04	$Q \rightarrow \sigma$
05	if ($\partial_{\mathcal{X}}(\sigma) = \{\beta\}$)
06	$\mathcal{X} = \mathcal{X} \setminus \{\sigma\}$
07	$Q \leftarrow \delta_{\mathcal{X}}(\beta)$
08	$\mathcal{X} = \mathcal{X} \setminus \{\beta\}$
09	else if ($\partial_{\mathcal{X}}(\sigma) = \emptyset$)
10	$Q \leftarrow \delta_{\mathcal{X}}(\beta)$
11	end if
12	end while
13	return \mathcal{X}

X is a Torus (70 vertices, 123 edges, 54 squares)

Goal: Construct a large acyclic set A



$C(X,A)$ generated by 19 edges, 16 squares

Run Times co-reduce

Random cubical complexes in \mathbb{R}^4

Size	$\beta_0, \beta_1, \beta_2$	Time
62,636	24, 2988, 20	0.53
116,284	36, 5552, 38	1.06
168,750	48, 8060, 54	1.56
222,480	54, 10493, 71	2.09

3.6 GHz PC
Pentium 4 processor
2 GB RAM

Large and high complexes

Dim.	Size	Betti	Time
3	8,392,997	1, 1057	4.38
4	350,000,000	1, 7, 352	935
12	135,351	1, 0, 0, 1, 4, 5, 0	0.77
12	332,309	1, 0, 0, 0, 0, 1, 1	1.92

Summary: The goal

Input: Large Geometrical Complex

Output: Small/Simple Chain Complex

3. Maps

A. Chain Maps (Algebra)

B. Approximating Continuous Maps

C. Constructing Chain Maps

D. Geometric Reductions

A. Chain Maps (Algebra)

Let $\mathcal{C} = \{C_k, \partial_k\}$ and $\mathcal{C}' = \{C'_k, \partial'_k\}$ be chain complexes.

A sequence of abelian group homomorphisms

$\varphi_k : C_k \rightarrow C'_k$ is a **chain map** if, for every $k \in \mathbb{Z}$,

$$\partial'_k \varphi_k = \varphi_{k-1} \partial_k.$$

Proposition: If $\varphi : \mathcal{C} \rightarrow \mathcal{C}'$ is a chain map, then

$$\varphi_k(Z_k) \subset Z'_k$$

$$\varphi_k(B_k) \subset B'_k$$

for all $k \in \mathbb{Z}$.

Define the group homomorphisms $\varphi_{k*} : H_k(\mathcal{C}) \rightarrow H_k(\mathcal{C}')$ by

$$\varphi_{k*}([z]) := [\varphi_k(z)]$$

B. Approximating Continuous Maps

Consider a continuous map $f : (X, A) \rightarrow (Y, B)$

Need to construct a chain map $f_{\#} : C_*(X, A) \rightarrow C_*(Y, B)$

First Question:

Consider $X \subset \mathbb{R}^n$, $Y \subset \mathbb{R}^m$. Let $x \in X$. What is $f(x)$?

1. Consider a differential equation $\dot{x} = g(x)$

which generates a flow $\psi : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$.

A natural continuous map is $f(x) := \psi(1, x)$.

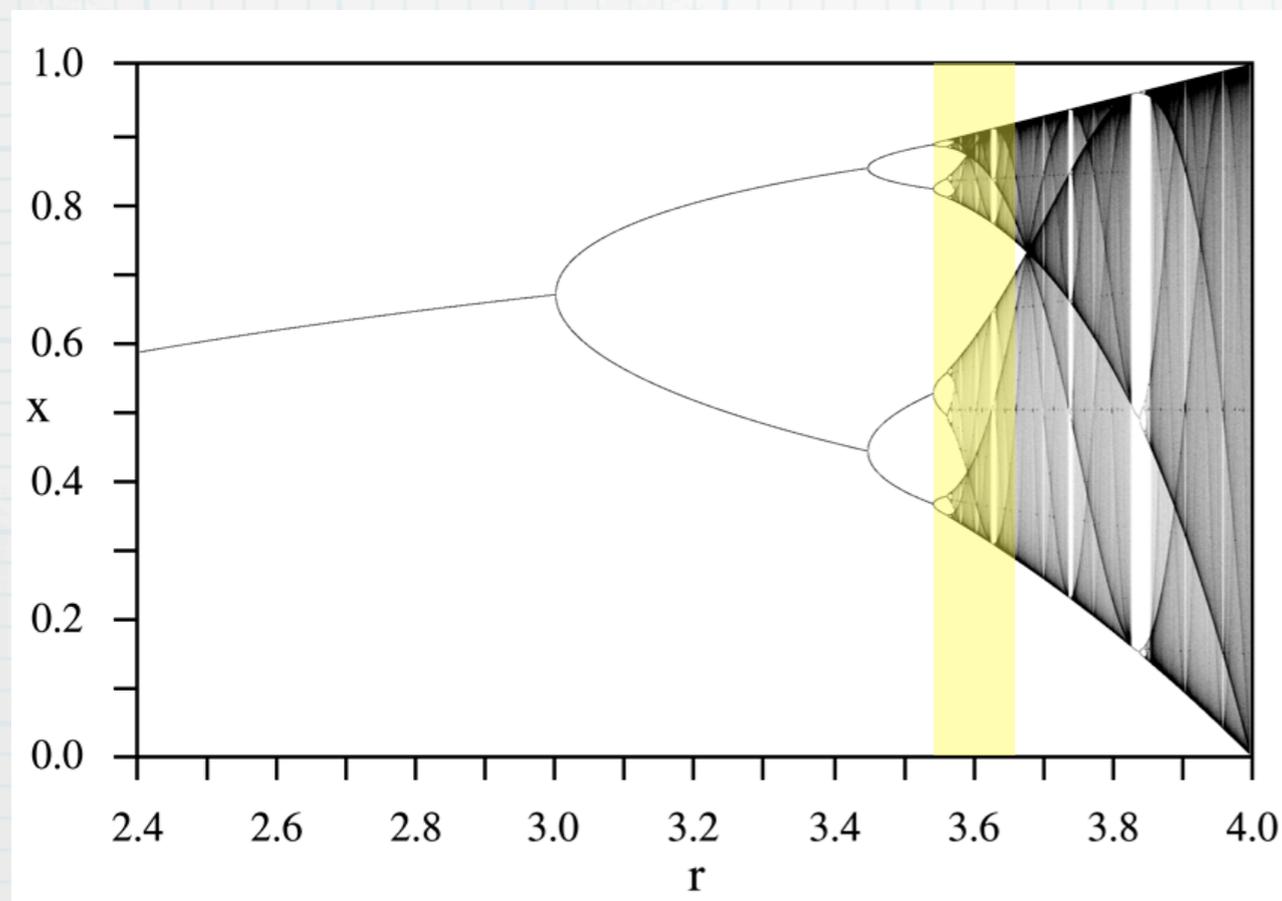
$f(x)$ is obtained by numerically integrating ode.

Cost of Integration vs. Numerical Errors

2. Consider a parameterized family of maps

$$f : X \times \Lambda \rightarrow X$$

Want to study dynamics over a set $Q \subset \Lambda$ of parameter values



Example: The Logistic Map

$$f(x, r) = r \cdot x \cdot (1 - x)$$

Explicit nonlinearities may give misleading information

$f(x, Q)$ is the minimal object of interest.

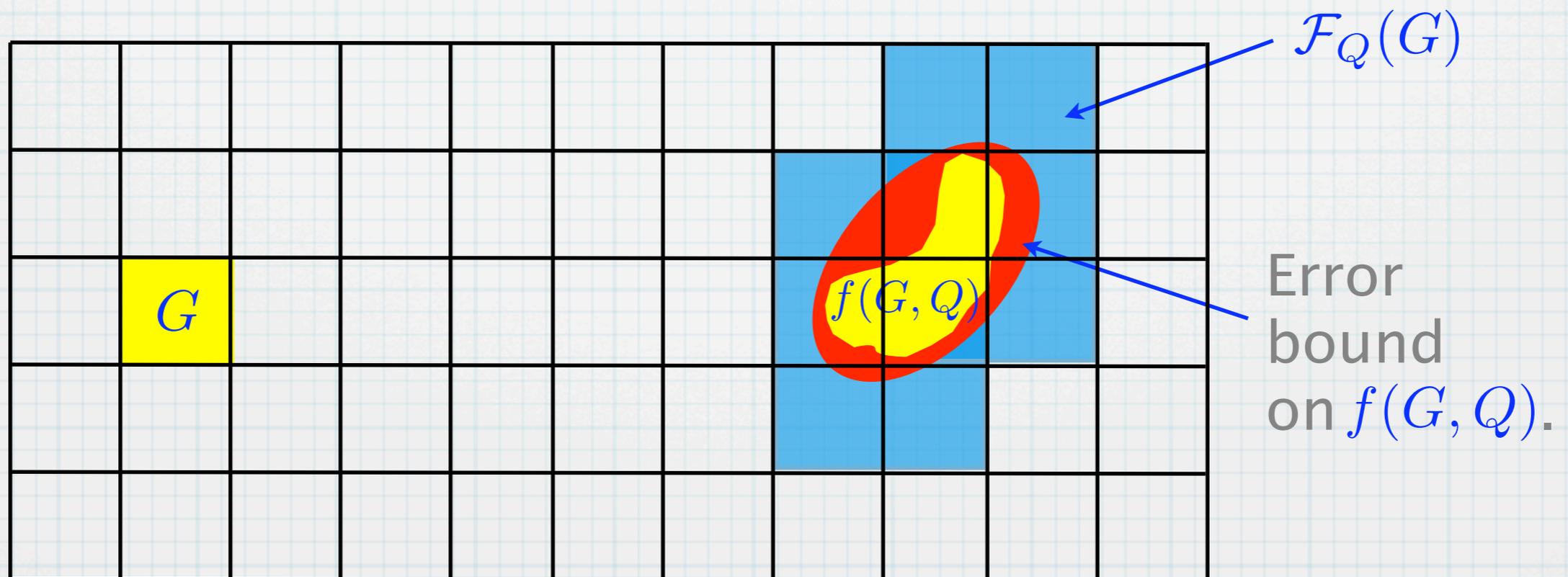
Constructing an acyclic multivalued approximation

Consider $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$. Accounting for errors

$$x \mapsto [f_1(x) - \epsilon, f_1(x) + \epsilon] \times [f_2(x) - \epsilon, f_2(x) + \epsilon]$$

Choose a cubical grid \mathcal{X} that covers X .

Construct a combinatorial multivalued map $\mathcal{F}_Q : \mathcal{X} \rightrightarrows \mathcal{X}$.



C. Constructing Chain Maps and Homology

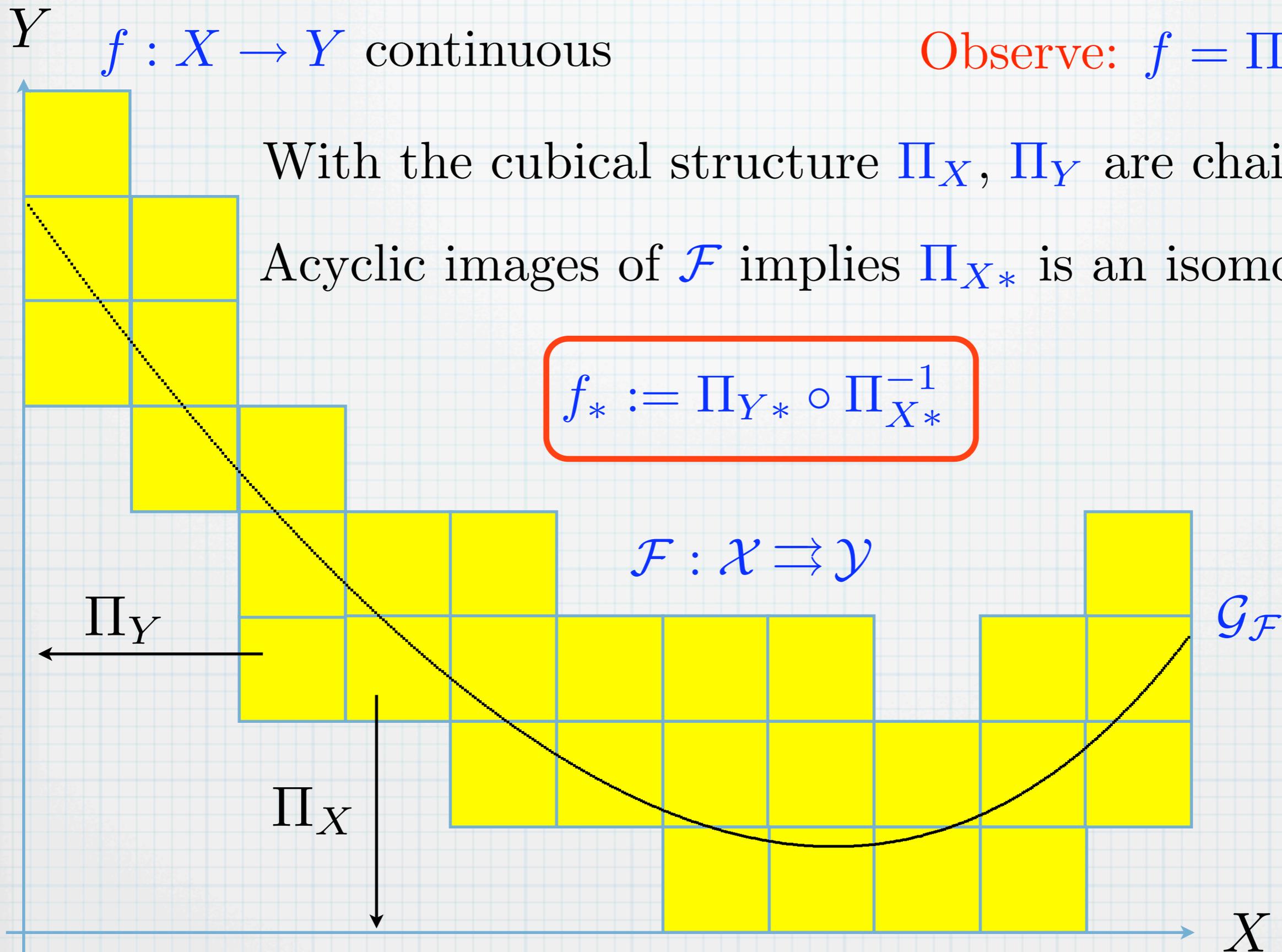
$f : X \rightarrow Y$ continuous

Observe: $f = \Pi_Y \circ \Pi_X^{-1}$

With the cubical structure Π_X, Π_Y are chain maps.

Acyclic images of \mathcal{F} implies Π_{X*} is an isomorphism.

$$f_* := \Pi_{Y*} \circ \Pi_{X*}^{-1}$$

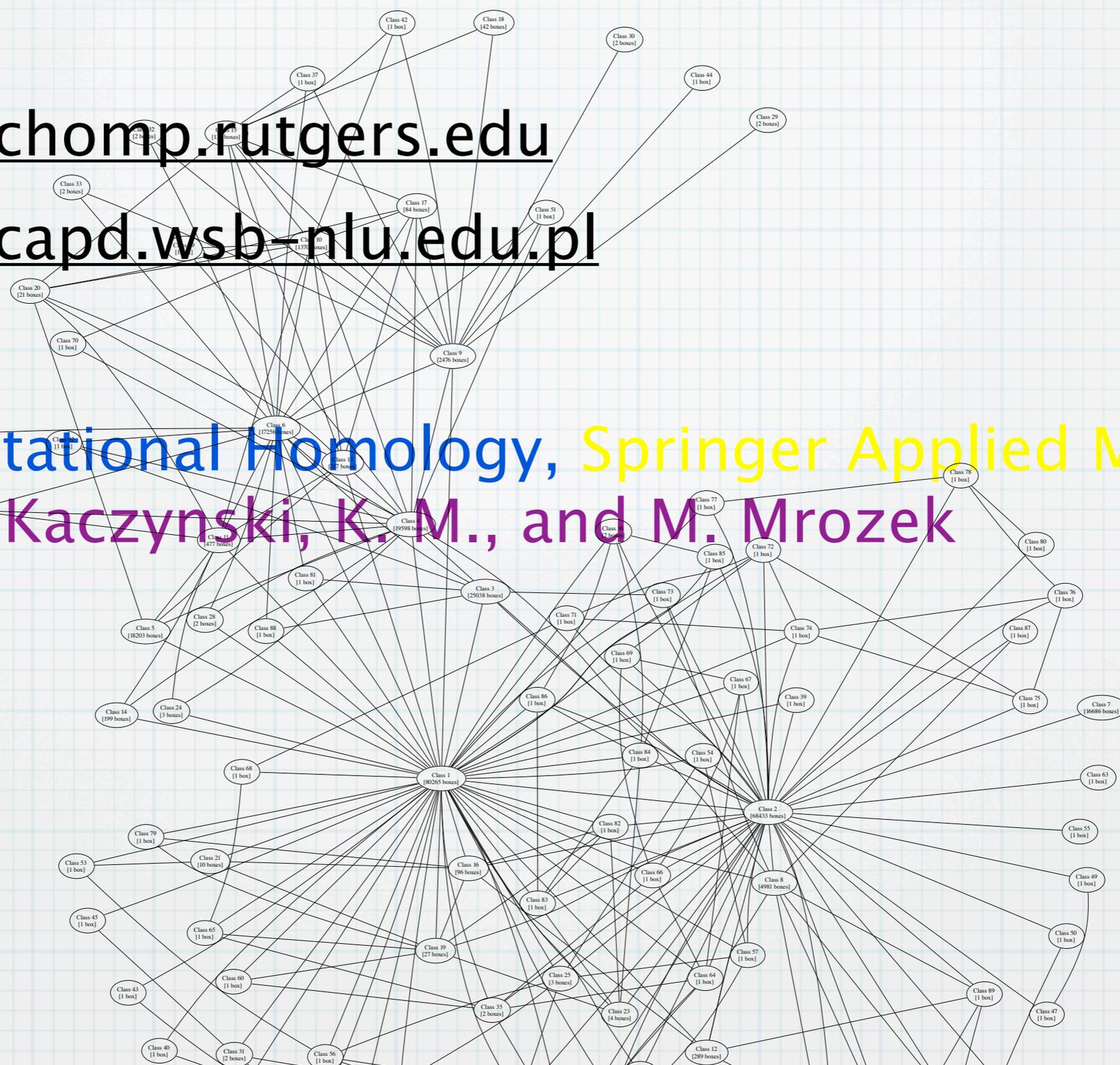


<http://chomp.rutgers.edu>

<http://capd.wsb-nlu.edu.pl>

Computational Homology, Springer Applied Math

T. Kaczynski, K. M., and M. Mrozek



National Science Foundation
WHERE DISCOVERIES BEGIN



U.S. DEPARTMENT OF
ENERGY