Rigorous Numerics in Dynamics: Validation of the Computations

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Recap

Bill Kalies: 1) There exist combinatorial/algebraic structures (Posets and Lattices) that organize asymptotic/invariant dynamics.

2) Given a dynamical system these combinatorial structures are computable.

Tomas Gedeon: 1) For multiscale problems or data-driven modeling analytic representations of dynamical system are not known.

2) Combinatorial/algebraic structures can be used to identify robust structures of dynamics over large ranges of parameter space (DSGRN).

This talk: 0) It is extremely useful (computationally, theoretically) to frame dynamics in this combinatorial/algebraic language.

1) Combinatorial/algebraic structures can be identified with analytic models.

2) Algebraic topology can be used to provide rigorous descriptions of dynamics.

Topology

and

Approximation

Let X be a compact metric space.

phase space

$f : X \to X$ continuous map

$\varphi : [0, \infty) \times X \to X$ semiflow

(unknown) dynamical system

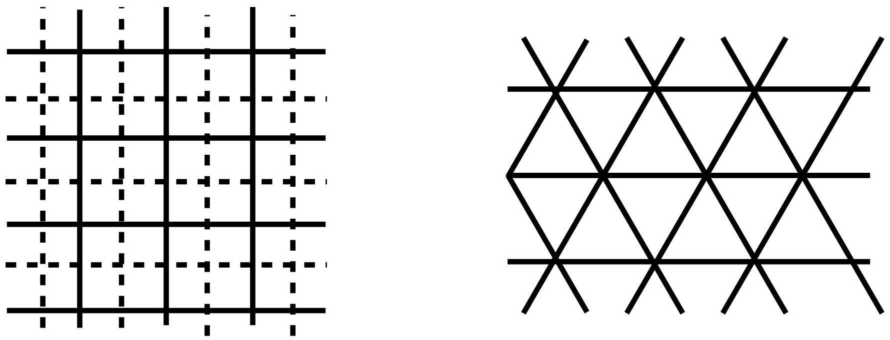
Let R(X) denote the lattice of regular closed subsets of X.

A is regular closed if $\mathrm{cl}(\mathrm{int}(A)) = A$

$A \vee B := A \cup B$

$A \wedge B := \mathrm{cl}(\mathrm{int}(A \cap B))$

Uncountable lattice
(space of approximations)



Let L be a finite bounded sublattice of R(X).

Level of measurement
Applicable scale for model

$\mathcal{X}(L)$ denotes atoms of L

"smallest" elements of **L**

Dynamics

Let L be a finite bounded sublattice of $\mathsf{R}(X)$ with atoms $\mathcal{X}(\mathsf{L})$

The lattice of attractors A is a bounded sublattice of L.

This is a combinatorial object

Bill's talk: from dynamics f outer approximation $\mathcal{F}\colon \mathcal{X}(\mathsf{L}) \rightrightarrows \mathcal{X}(\mathsf{L})$ to A.

Tomas' talk: from $\mathcal{F}\colon \mathcal{G}(\mathsf{L}) \rightrightarrows \mathcal{G}(\mathsf{L})$ ($\mathcal{G}(\mathsf{L})$ a cell complex generated by $\mathcal{X}(\mathsf{L})$) to A.

Questions: How do we identify models with this information?
How do we extract structures associated with classical dynamics from this information?

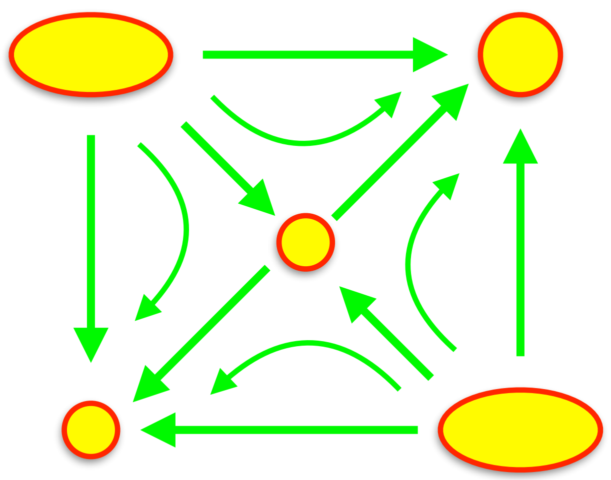
Recall: Given a bounded distributive lattice A, $A \in \mathsf{A}$ is join irreducible if it has a unique immediate predecessor ($A = B \vee C$ implies $A = B$ or $A = C$).

The set of join irreducible elements $\mathsf{J}^{\vee}(\mathsf{A})$ forms a poset $(\mathsf{P}, <)$.

Extracting Dynamics
from
DSGRN

Classical dynamics: dynamics is describe in terms of invariant sets

(C. Conley) A Morse decomposition of a compact invariant set S consists of a finite collection of mutually disjoint compact invariant subsets $M(p)$ labeled by a poset $(\mathsf{P}, <)$ such that if

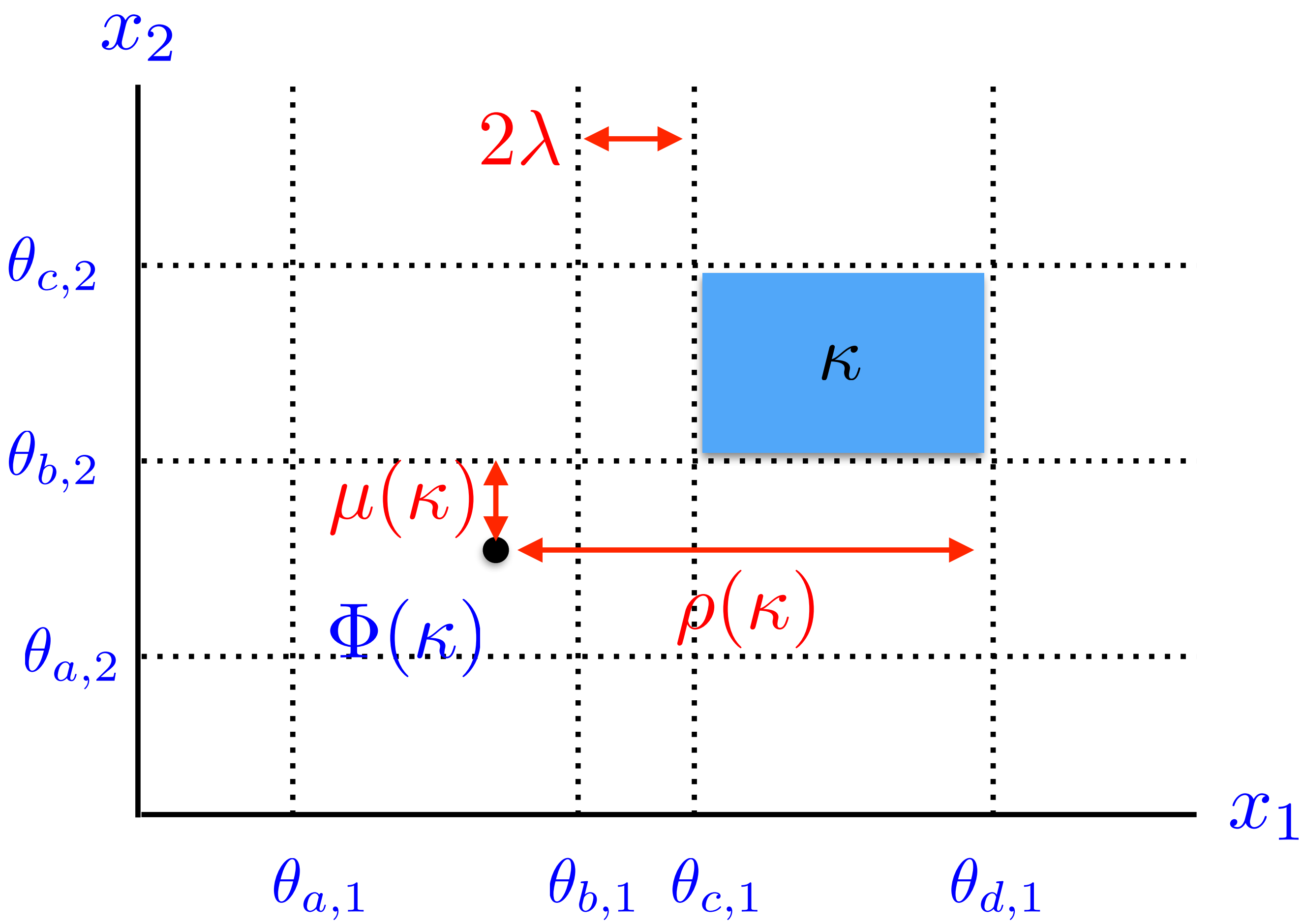


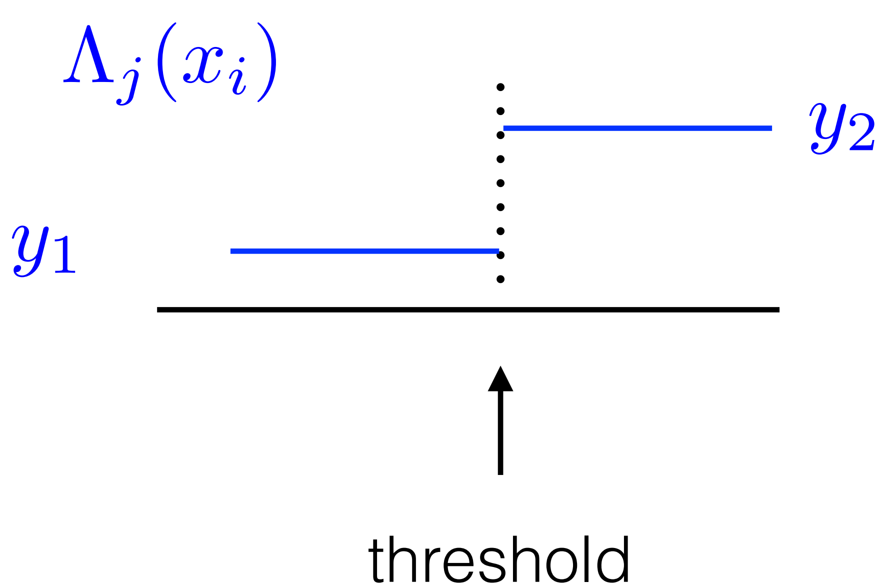
$$x \in S \setminus \bigcup_{p \in \mathsf{P}} M(p)$$

then there exists $q > p$ such that

$$\alpha(x) \subset M(q) \quad \text{and} \quad \omega(x) \subset M(p).$$

Generalized 2-D DSGRN





Set

$$\Phi(\kappa) := \begin{pmatrix} \gamma_1^{-1}\Lambda_1(\kappa) \\ \gamma_2^{-1}\Lambda_2(\kappa) \end{pmatrix}$$

Define:

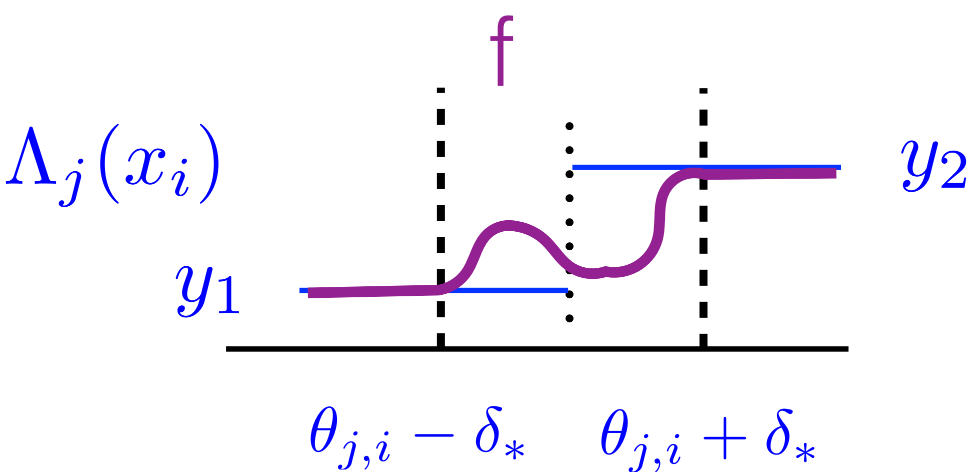
$$\mu = \min_{\kappa} \mu(\kappa)$$

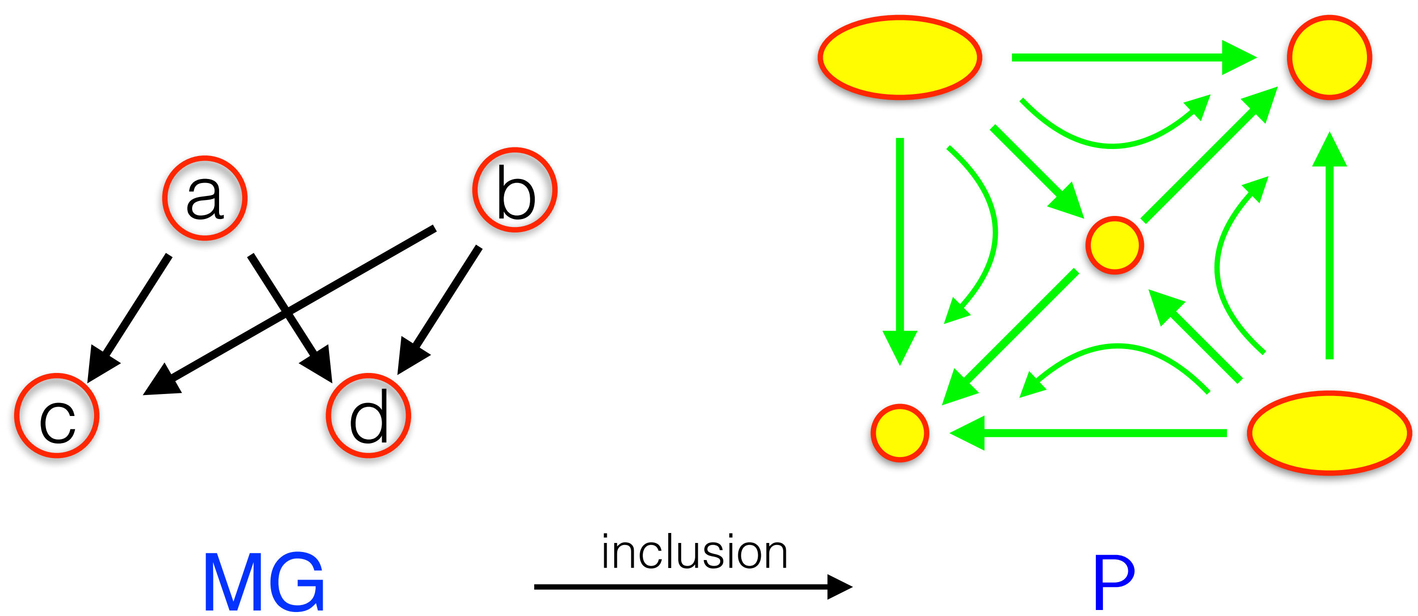
$$\rho = \max_{\kappa} \rho(\kappa)$$

$$\bar{\gamma} = \min\left\{\frac{\gamma_1}{\gamma_2}, \frac{\gamma_2}{\gamma_1}\right\}$$

$$\delta_* := \min\left\{\frac{\lambda\mu\bar{\gamma}}{\sqrt{2}(2\lambda+3\rho)}, \sqrt{\frac{\lambda\mu\bar{\gamma}}{32}}\right\}$$

Theorem: (T. Gedeon, S. Harker, H. Kokubu, K.M., H. Oka) Let $(\mathrm{MG}, <)$ be the poset associate with a Morse graph computed using DSGRN at a parameter value $(\ell, u, \theta, \gamma) \in (0, \infty)^{2+3\cdot\#\text{thresholds}}$.





Moral: DSGRN rigorously captures dynamics of large classes of models.

Identifying Dynamical Systems from Lattice Structures

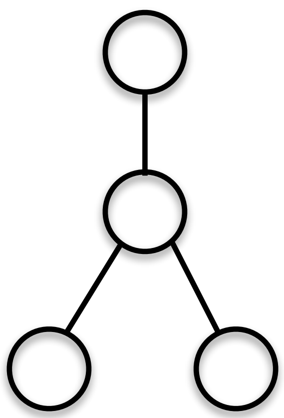
Example I

Phase space: $X = [-4, 4] \subset \mathbb{R}$

Atoms of lattice $\mathcal{X}(\mathsf{L}) = \{[n, n+1] \mid n = -4, \ldots, 3\}$

Lattice of attractors: $\mathsf{A} = \{[-3,-1], [1,3], [-3,-1] \cup [1,3], [-4,4]\}$

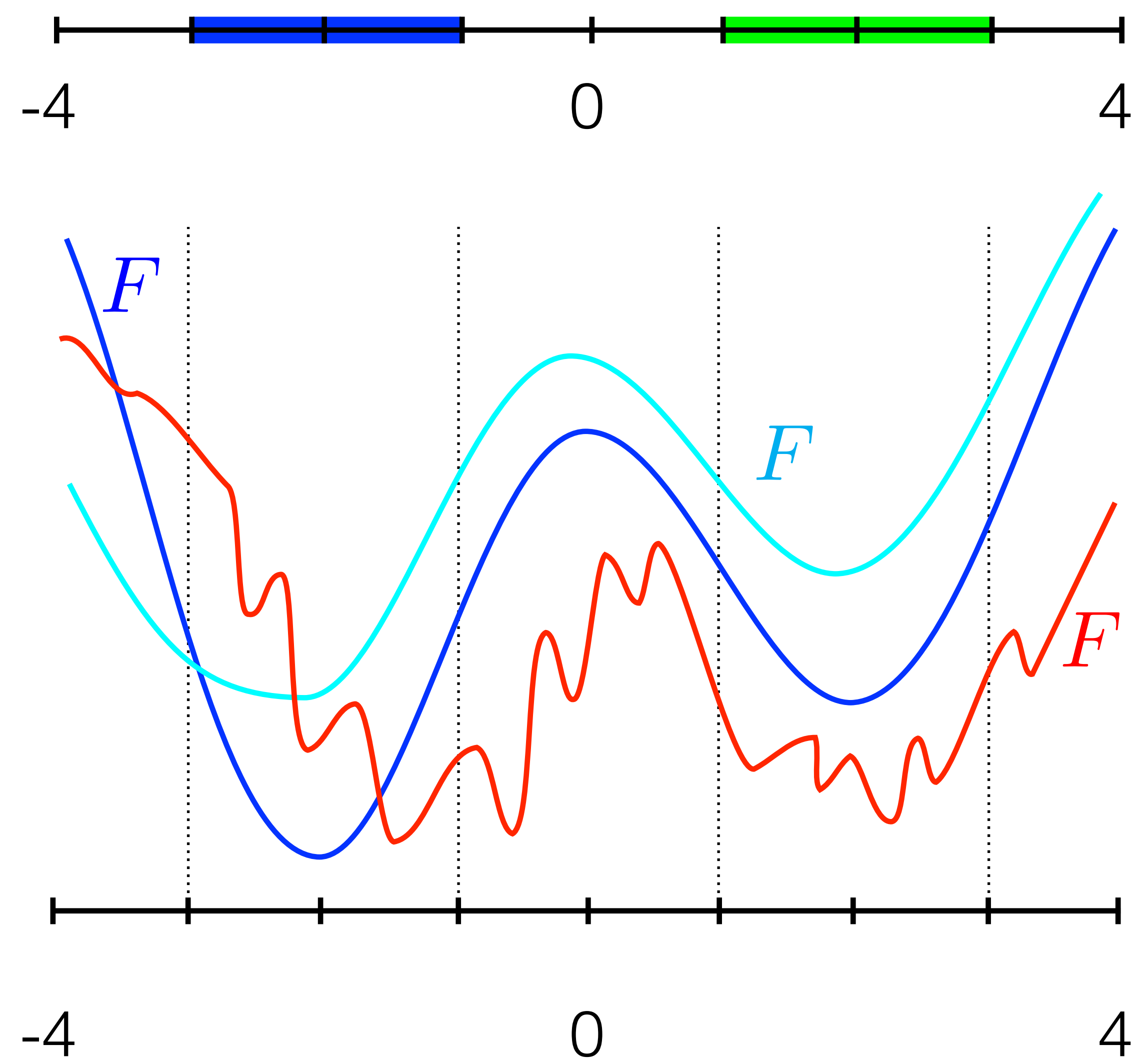
A



How does this relate to a differential equation $\frac{dx}{dt} = f(x)$?

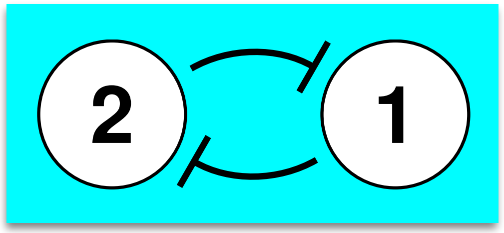
Let $F'(x) = -f(x)$.

Combinatorial attractors represent regions of phase space that are forward invariant with time.



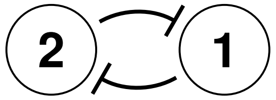
Example II (Toggle Switch via DSGRN)

Input:
Regulatory Network



Output:
DSGRN database

(1) FP(0,1): $u_{1,2} < \gamma_1\theta_{2,1}$, $\gamma_2\theta_{1,2} < l_{2,1}$	(2) FP(0,1): $u_{1,2} < \gamma_1\theta_{2,1}$, $l_{2,1} < \gamma_2\theta_{1,2} < u_{2,1}$	(3) FP(0,0): $u_{1,2} < \gamma_1\theta_{2,1}$, $u_{2,1} < \gamma_2\theta_{1,2}$
(4) FP(0,1): $l_{1,2} < \gamma_1\theta_{2,1} < u_{1,2}$, $\gamma_2\theta_{1,2} < l_{2,1}$	(5) FP(0,1) FP(1,0): $l_{1,2} < \gamma_1\theta_{2,1} < u_{1,2}$, $l_{2,1} < \gamma_2\theta_{1,2} < u_{2,1}$	(6) FP(1,0): $l_{1,2} < \gamma_1\theta_{2,1} < u_{1,2}$, $u_{2,1} < \gamma_2\theta_{1,2}$
(7) FP(1,1): $\gamma_1\theta_{2,1} < l_{1,2}$, $\gamma_2\theta_{1,2} < l_{2,1}$	(8) FP(1,0): $\gamma_1\theta_{2,1} < l_{1,2}$, $l_{2,1} < \gamma_2\theta_{1,2} < u_{2,1}$	(9) FP(1,0): $\gamma_1\theta_{2,1} < l_{1,2}$, $u_{2,1} < \gamma_2\theta_{1,2}$



DSGRN

$$\dot{x}_1 = -\gamma_1 x_1 + \ell_{1,2} + \frac{u_{1,2} - \ell_{1,2}}{\theta_{1,2}^n + x_2^n}$$

$$\dot{x}_2 = -\gamma_2 x_2 + \ell_{2,1} + \frac{u_{2,1} - \ell_{2,1}}{\theta_{2,1}^n + x_1^n}$$

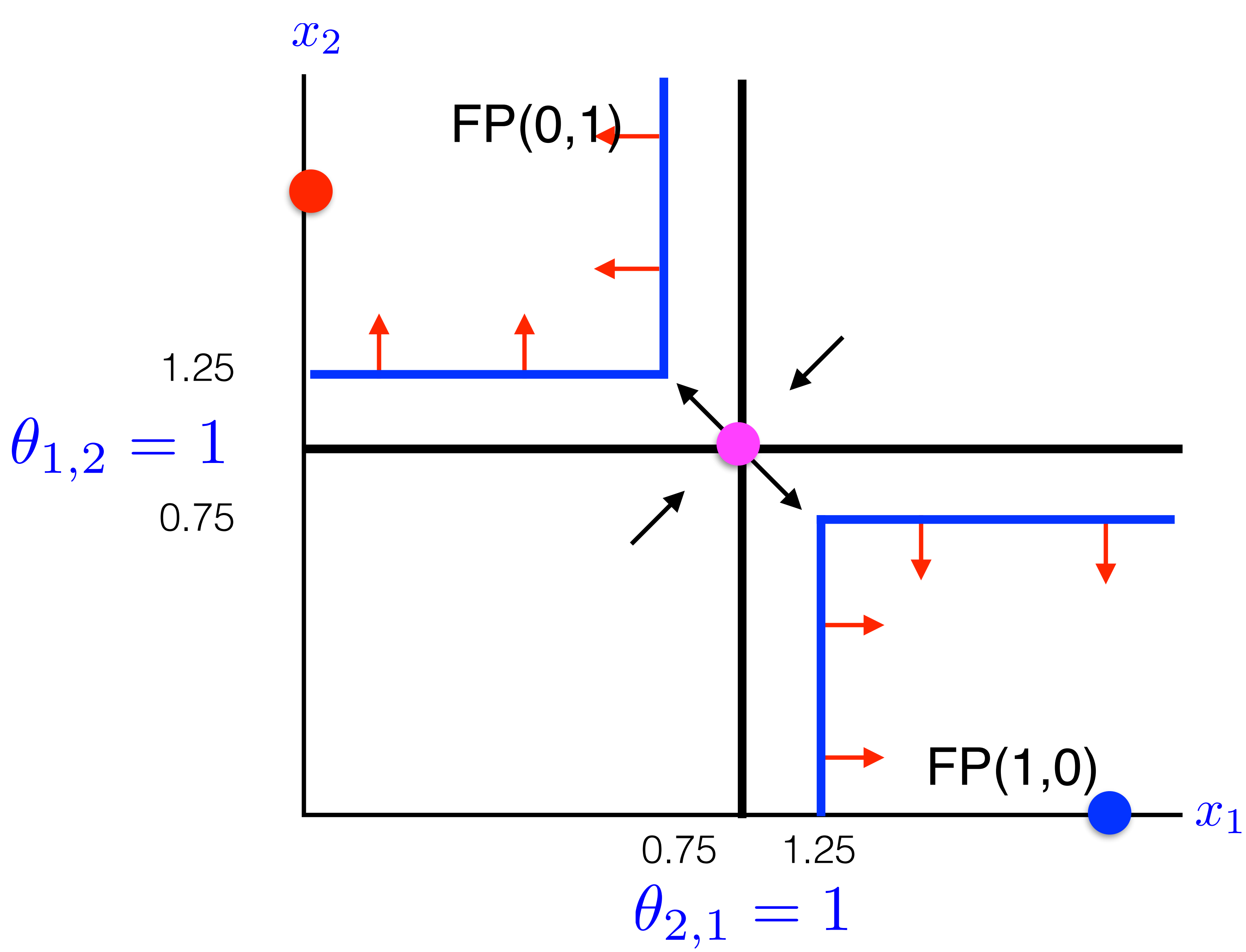
Hill function model

Choose parameter values

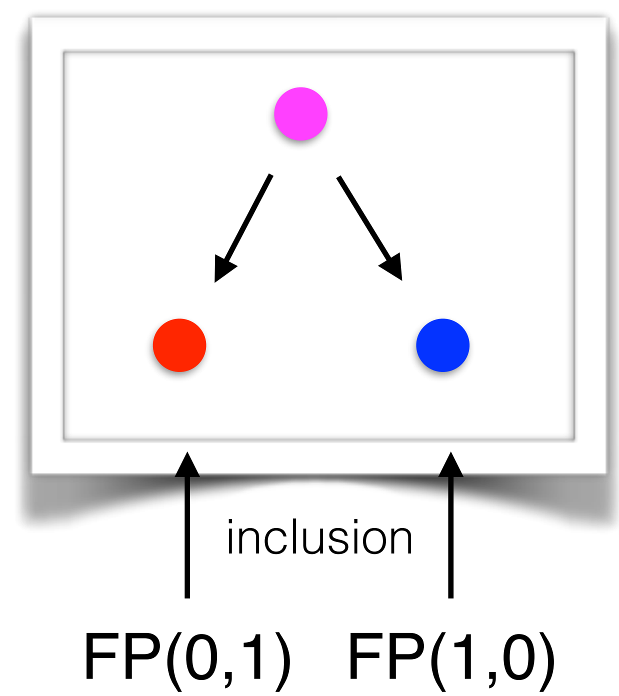
$$\dot{x}_1 = -x_1 + \frac{2}{1 + x_2^n}$$

$$\dot{x}_2 = -x_2 + \frac{2}{1 + x_1^n}$$

	FP(0,1) FP(1,0)
(5)	$l_{1,2} < \gamma_1 \theta_{2,1} < u_{1,2}$
	$l_{2,1} < \gamma_2 \theta_{1,2} < u_{2,1}$



Poset for a Morse decomposition for the flow



For $n \geq 4.5$ vector field is transverse to blue regions.

Extracting Dynamics from Outer Approximations (DSGRN)

$\mathsf{A} \subset \mathsf{L}$ is a lattice of attractors.

Use Birkhoff to define poset $(\mathsf{P} := \mathsf{J}^{\vee}(\mathsf{A}), <)$

For each $p \in \mathsf{P}$ define a Morse tile $\mathsf{M}(p) := \mathrm{cl}(A \setminus \mathsf{pred}(A))$

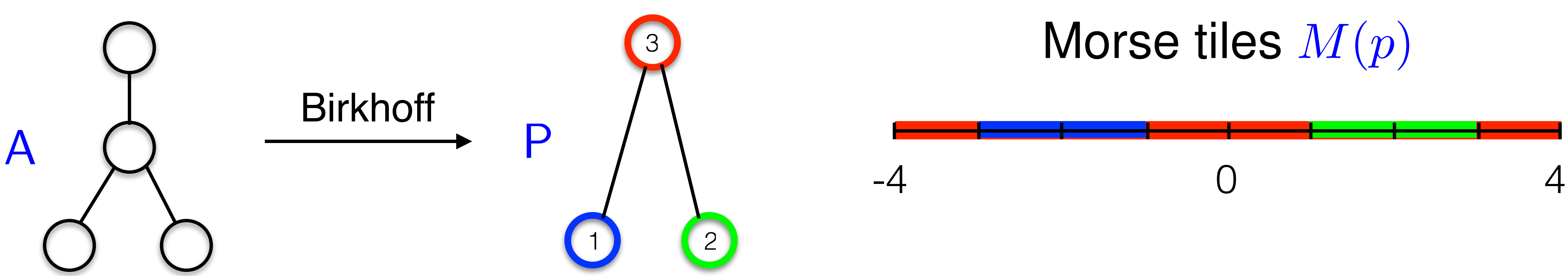
Recall Example

Phase space: $X = [-4, 4] \subset \mathbb{R}$

$\mathsf{A} \subset \mathsf{L}$ is a lattice of attractors.

Atoms of lattice $\mathcal{X}(\mathsf{L}) = \{[n, n+1] \mid n = -4, \ldots, 3\}$

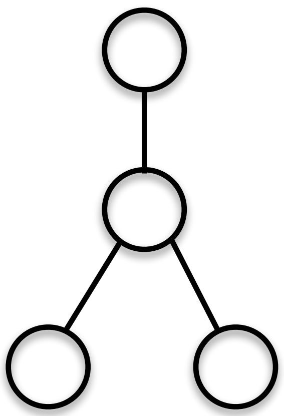
Lattice of attractors: $\mathsf{A} = \{[-3, -1], [1, 3], [-3, -1] \cup [1, 3], [-4, 4]\}$



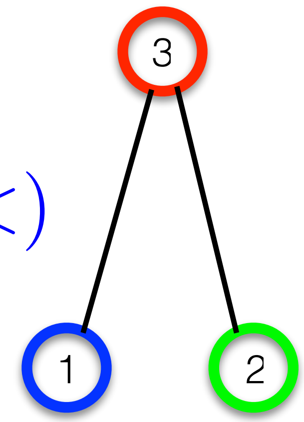
EXAMPLE (CONTINUED)

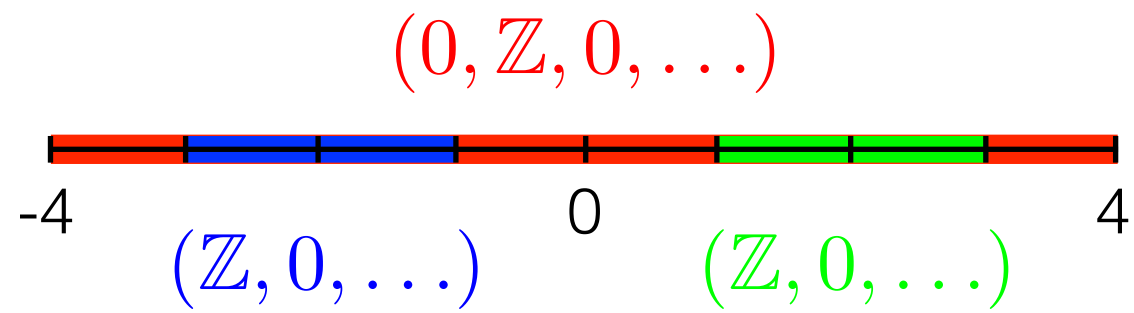
$X = [-4, 4] \subset \mathbb{R}$

A



(P, <)





For flows the homology Conley index of M(p) is

$$CH_*(p) := H_*(A, \text{pred}(A))$$

For maps the homology Conley index of M(p) is the shift equivalence class of

$$f_*\colon H_*(A, \text{pred}(A)) \to H_*(A, \text{pred}(A))$$

Remark: f_* can be computed (rigorously) from an outer approximation $\mathcal{F}\colon \mathcal{X}(\mathsf{L}) \rightrightarrows \mathcal{X}(\mathsf{L})$ without knowing f.

S. Harker, K.M., M. Mrozek, V. Nanda, FoCM, 2013

S. Harker, H. Kokubu, K.M., P. Pilarczyk, Proc. AMS, 2016

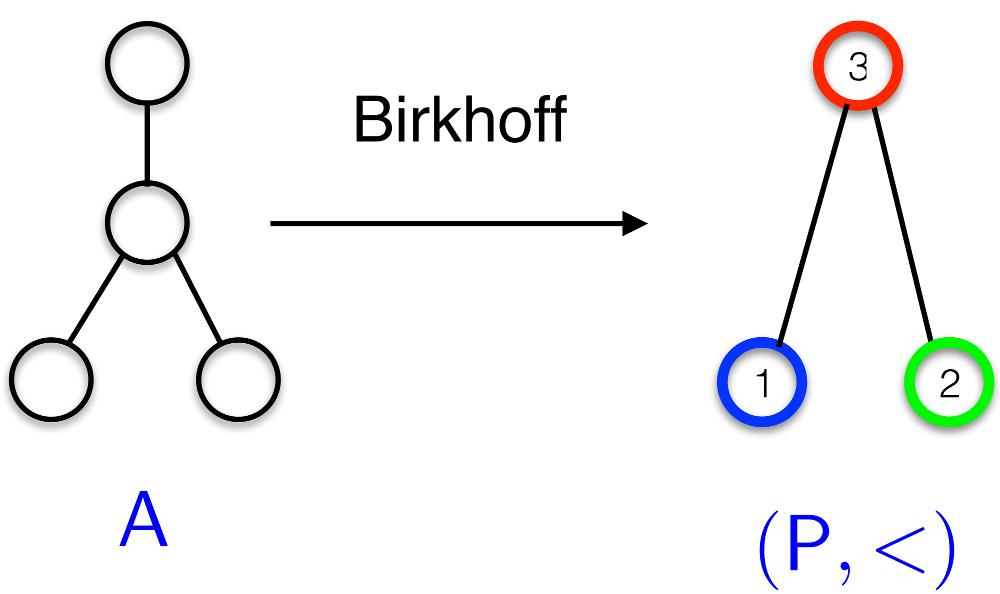
Theorem: (C. Conley; M. Mrozek; J. Robbin, D. Salamon) If Conley index of the Morse tile $M(p)$ is nontrivial, then there exists a non-empty invariant set in $\mathrm{cl}(A \setminus \mathrm{pred}(A))$.

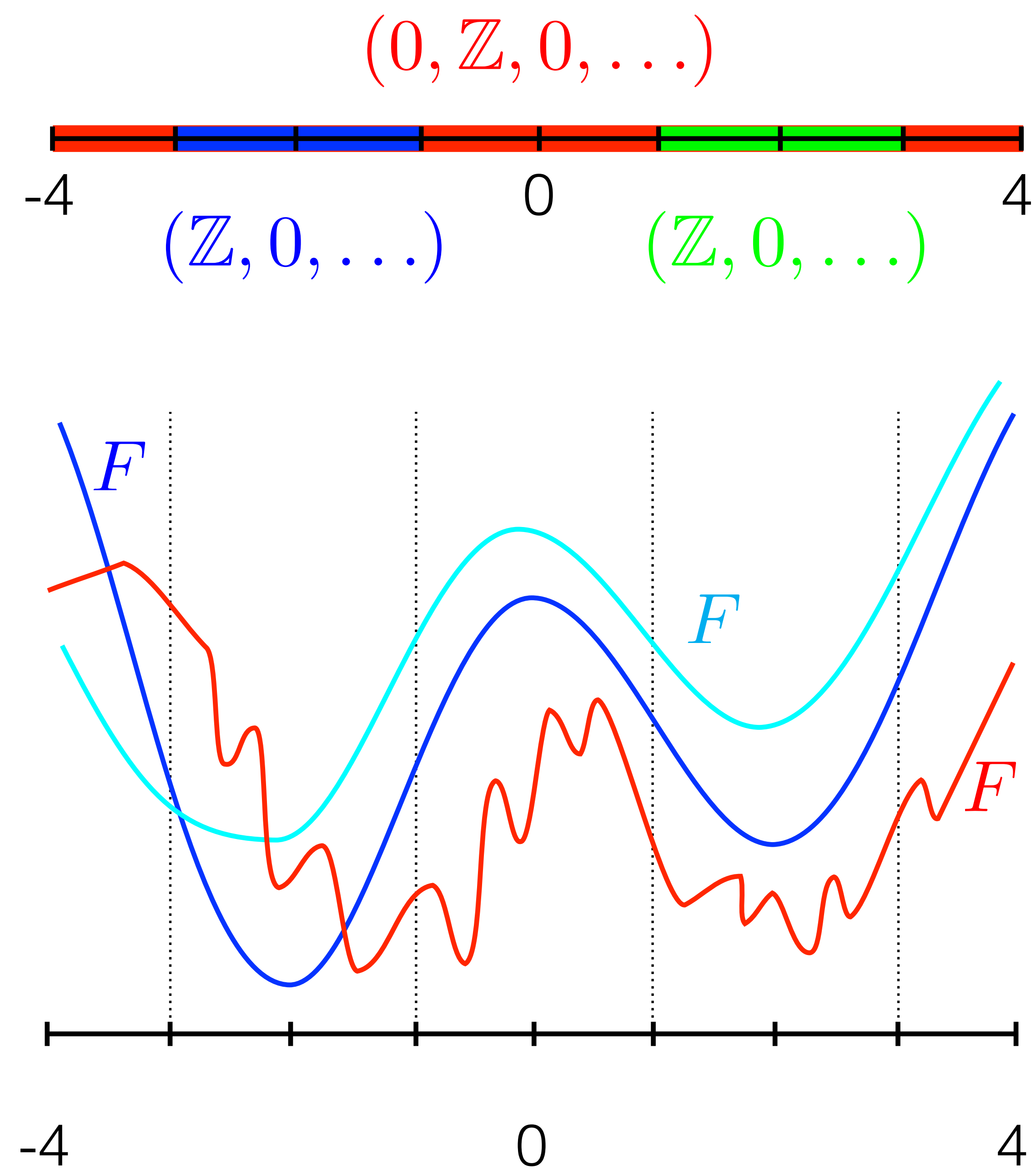
Recall Example:

Phase space: $X = [-4, 4] \subset \mathbb{R}$

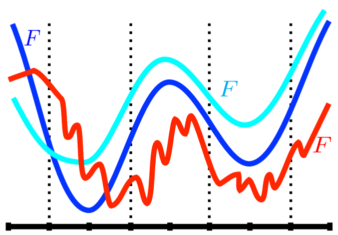
Lattice of Attractors

$\mathsf{A} = \{[-3,-1], [1,3], [-3,-1] \cup [1,3], [-4,4]\}$





Moral: We can make nontrivial statements about dynamics without having an analytic representation of the dynamical system.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F
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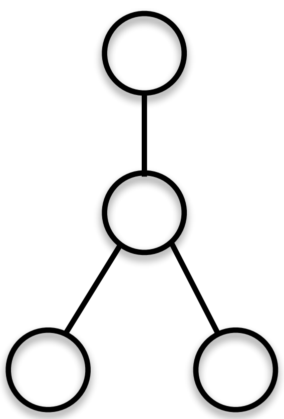
Conley index can be used to guarantee existence of equilibria, periodic orbits, heteroclinic and homoclinic orbits, and chaotic dynamics.

Theorem: (R. Franzosa) There exists a strictly upper triangular (with respect to $<$) boundary operator

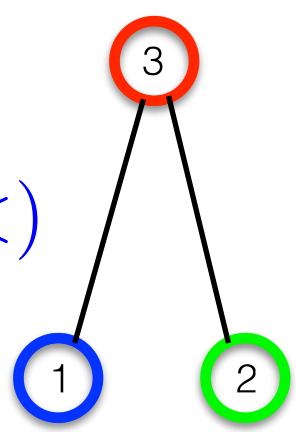
$$\Delta : \bigoplus_{p \in \mathsf{P}} CH_*(p) \to \bigoplus_{p \in \mathsf{P}} CH_*(p)$$

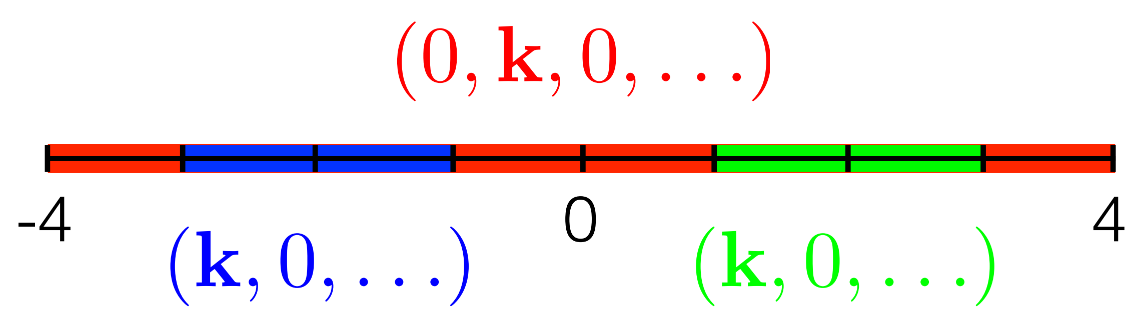
such that the induced homology is isomorphic to $H_*(X)$.

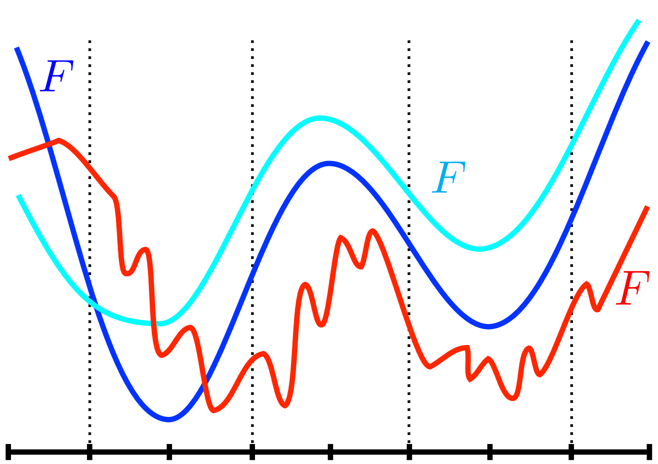
A



(P, <)







$$\Delta = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} : \bigoplus_{p=1}^{3} CH_*(p) \to \bigoplus_{p=1}^{3} CH_*(p)$$

Claim: (S. Harker, K. Spendlove, K.M.)
Δ can be computed efficiently.

Thank-you for your Attention

W. Kalies, Florida Atlantic U.
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T. Gedeon, Montana State
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H. Oka, Ryukoku U.

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