

An Operadic Approach to Compositionality

David I. Spivak

dspivak@math.mit.edu
Mathematics Department
Massachusetts Institute of Technology

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Simons Institute for the Theory of Computing

Outline

- 1 Introduction
- 2 Operads of string diagrams
- 3 Steady states are compositional
- 4 Conclusion

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1 Introduction

- What is compositionality?
- Plan of the talk

2 Operads of string diagrams

3 Steady states are compositional

4 Conclusion

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 - We should specify not only the **pieces**, but also their **arrangement**.
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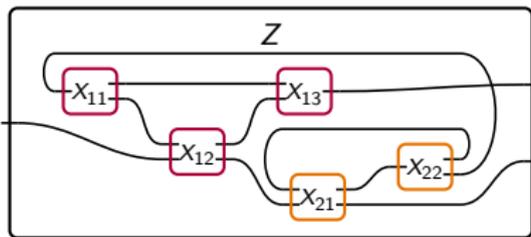
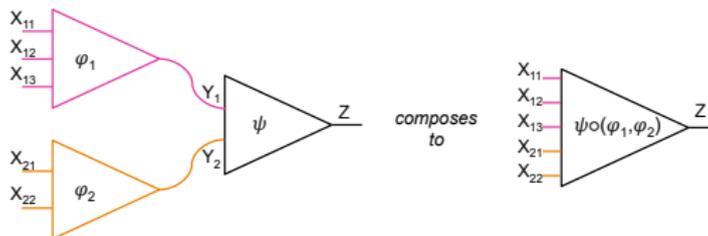
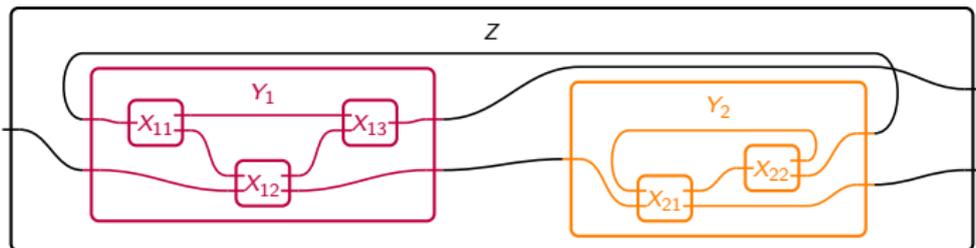
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 - Arrangements can be **nested** inside each other.
- This leads naturally to the notion of operad \mathcal{O} , which specifies:
 - the set of possible **things** X, Y, \dots ;
 - the set of **arrangements** φ, ψ by which one thing is composed of many;
 - how **nesting** works $\psi \circ (\varphi_1, \dots, \varphi_n)$.

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- Note: by *operad*, I mean what is usually called “**colored operad**”.

Picturing arrangements φ, ψ of things X, Y, Z



Syntax and semantics

- An operad \mathcal{O} specifies a *theory of composition*.
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 - These are the **sorts** and the **operations** in our theory \mathcal{O} of composition.
- Functorial semantics: a *model of \mathcal{O}* is a functor $M: \mathcal{O} \rightarrow \mathbf{Set}$.
 - For every **sort** $X \in \mathcal{O}$, we have a set $M(X)$ of things of that sort.
 - For every **arrangement** $\varphi: X_1, \dots, X_n \rightarrow Y$ in \mathcal{O} , we have a function

$$M(\varphi): M(X_1) \times \dots \times M(X_n) \rightarrow M(Y).$$
 - Given a tuple $(x_1, \dots, x_n) \in M(X_1) \times \dots \times M(X_n)$,
 - and a rule φ for assembling them,
 - we obtain some new $\varphi(x_1, \dots, x_n) \in M(Y)$.
- I think this is a reasonable formalism for the term *composition*.

What is compositionality?

In my lexicon, it is *attributes* and *analyses* that can be compositional.

- An attribute is like a projection onto a simpler space.
 - One attribute of an ODE is its set of steady states (subset of \mathbb{R}^n).
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- Formally, suppose given an operad \mathcal{O} and a model $M: \mathcal{O} \rightarrow \mathbf{Set}$.
 - By a *compositional analysis*, I mean a system of attributes for \mathcal{O} .
 - It consists of an \mathcal{O} -model N and a natural transformation $A: M \rightarrow N$.
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 - *Compositionality*: for any **arrangement** φ and **things** x_1, \dots, x_n , we have

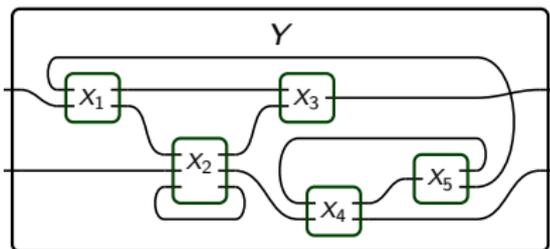
$$A_Y(M(\varphi)(x_1, \dots, x_n)) = N(\varphi)(A_{X_1}(x_1) \dots, A_{X_n}(x_n))$$

- Compositionality of A means the following two things are the same:
 - composing pieces in the model, then projecting via attribute A
 - projecting each piece via attribute A , then composing their images.
- Summary: “analyzing commutes with assembling.”

Example 1: steady states of dynamical systems

Taking steady states is a compositional analysis of dynamical systems.

- There is an operad \mathcal{W} for composing dynamical systems.

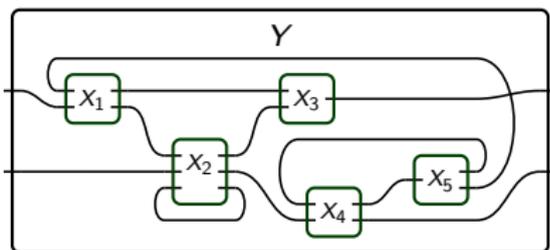


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- We'll discuss a model $DS: \mathcal{W} \rightarrow \mathbf{Set}$ of “dynamical systems”.
- There is a compositional analysis $A: DS \rightarrow \mathbf{Mat}$.
 - Here, $\mathbf{Mat}: \mathcal{W} \rightarrow \mathbf{Set}$ is the model of matrices.
 - A assigns to each dynamical system its matrix of steady states.
 - Compute steady states of composite system by matrix arithmetic.

Example 2: hierarchical protein materials

There is an operad \mathcal{M} for composing hierarchical protein materials.

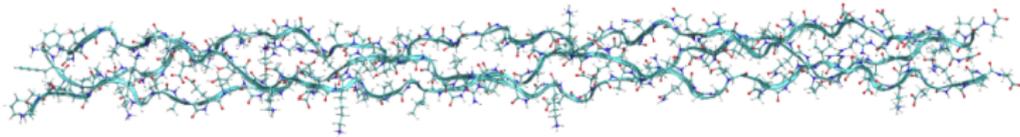
- A **protein** is an **arrangement** of simpler **proteins**.
 - There are atomic proteins, namely amino acids.
 - Protein materials include your skin: stretchable, breathable, waterproof.
 - (Computer MD versions of) proteins are a model, $\text{Prot}: \mathcal{M} \rightarrow \mathbf{Set}$.¹

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- A new protein can be assembled from a finite set of proteins
 - arranged in series or parallel, or
 - arranged in helices, double helices, any conceivable curve, etc.

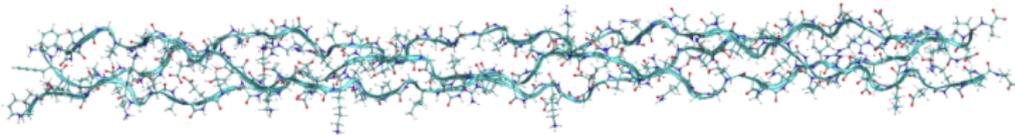


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- A compositional analysis would be “incredibly” useful in mat. sci.:
 - Example: assign a value, e.g. strength or toughness, to each protein
 - with a formula for composing strengths according to any arrangement.
 - Even if not perfectly compositional, it would be highly valuable.

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Plan of the talk

Here's the plan for the rest of the talk.

- Discuss operads of string diagrams. In particular:
 - monoids and categories,
 - traced monoidal categories,
 - hypergraph categories.
- Exemplify compositional analyses: steady states of dynamic systems.
 - Define dynamical system (continuous, discrete).
 - Define their steady states and show how they “compose like matrices”.
- Conclude with a few more words on compositionality (or lack thereof).

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 - Monoids and categories
 - Traced categories and cobordisms
 - Hypergraph categories
 - The real role of operads
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String diagrams

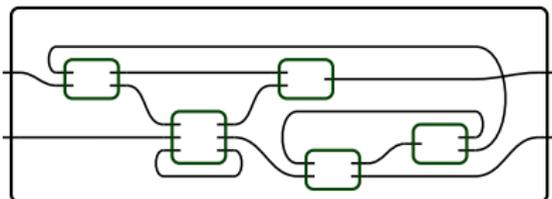
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 - We can organize the string diagrams for a doctrine as an operad \mathcal{O} .
 - The connection between string diagrams and their meaning is a functor $M: \mathcal{O} \rightarrow \mathbf{Set}$.

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- How operads come into play:
 - We can organize the string diagrams for a doctrine as an operad \mathcal{O} .
 - The connection between string diagrams and their meaning is a functor $M: \mathcal{O} \rightarrow \mathbf{Set}$.
- Below is an example string diagram for traced monoidal categories.

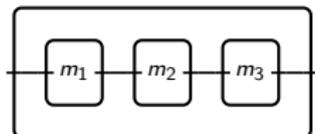


- We want to encode such diagrams as mathematical objects.

String diagrams for monoids

It is well-known that the terminal operad \mathcal{T} is the theory of monoids.

- \mathcal{T} has one object $*$, and one n -ary morphism for every n .
- A model of \mathcal{T} is (as always) a functor $M: \mathcal{T} \rightarrow \mathbf{Set}$.
 - It assigns to the unique object $*$ a set $M := M(*)$.
 - It assigns an operation $M^n = M \times \cdots \times M \rightarrow M$ for every n .

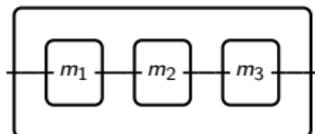


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- The composition formula in \mathcal{T} ensures the associativity and unitality.
- One can think of this as an “unbiased” perspective on monoids:
 - \mathcal{T} gives us all the operations (n -ary multiplication) on equal footing,
 - in contrast to the usual approach: two generators, unit and mult.

String diagrams for categories: monoids + labels

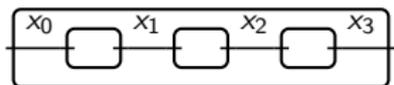
String diagrams focus on morphisms, not objects.

- This is the downside of using operads: they are parametric on objects.
 - So there is no operad for categories.
 - For any set of objects Λ , there is an operad for Λ -categories.
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 - I'd like a nice way to deal with this, but haven't settled on anything.
- Choose Λ . Define \mathcal{O}_Λ as the following operad.
 - Its objects are pairs $X = (x_1, x_2) \in \Lambda^2$, drawn $x_1 \square x_2$.
 - Its n -ary morphisms $X_1, \dots, X_n \rightarrow Y$ are tuples $(x_0, \dots, x_n) \in \Lambda^{n+1}$,
 - ... such that $X_i = (x_{i-1}, x_i)$ and $Y = (x_0, x_n)$.



- A model $\mathcal{C}: \mathcal{O}_\Lambda \rightarrow \mathbf{Set}$ is an (“unbiased”) category with objects Λ :
 - \mathcal{C} assigns a set $\mathcal{C}(x_1, x_2)$ to each object $(x_1, x_2) \in \Lambda^2$
 - and assigns a “composition formula” to each compatible string of such.
- Next: there's a similar but more interesting story for traced categories.

Traced monoidal categories are models of *Cob*

Modulo string labels, the operad for traced monoidal categories is *Cob*:²

Theorem

There is an equivalence of categories: $\mathbf{Fun}(Cob, \mathbf{Set}) \simeq \mathbf{TrCat}$.

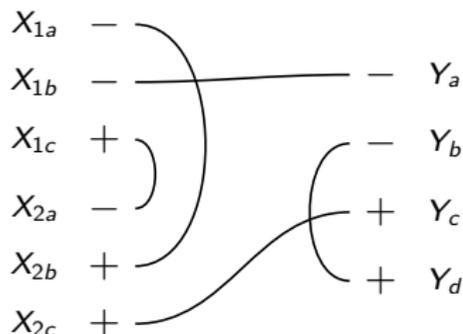
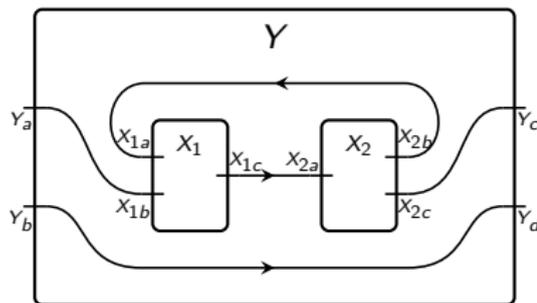
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Hypergraph categories

Another doctrine seems useful in applications: "hypergraph categories".

- The usual definition of *hypergraph category* is a bit "involved":
 - It is a symmetric monoidal category \mathcal{C} in which
 - each object is equipped with the structure of a monoid and comonoid
 - that satisfy several additional axioms.

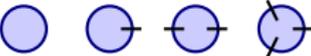
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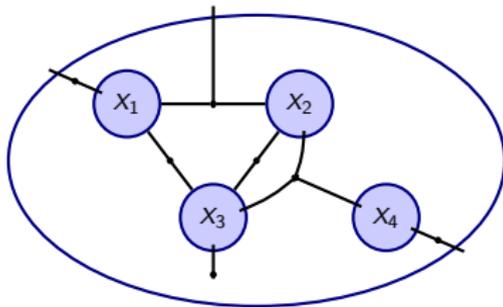
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But the concept is quite easy from the perspective of string diagrams.

- As indicated by the name, string diagrams are *hypergraphs*.
- Pictorially, \mathcal{H} is the operad with these objects and morphisms:

objects:  etc.

morphisms:



Operad $\mathcal{H} = \text{Cospan}$ and hypergraph categories

Let's give a more formal description of the operad \mathcal{H} .

- Different authors could mean slightly different things. Main issue:
- Can an edge in a hypergraph be incident to *zero* vertices?
 - If yes, then $\mathcal{H} = \text{Cospan}$.
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 - Morphisms are either cospans $X_1 \sqcup \cdots \sqcup X_n \rightarrow L \leftarrow Y$
 - or jointly surjective cospans $X_1 \sqcup \cdots \sqcup X_n \sqcup Y \twoheadrightarrow L$.

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- Examples of hypergraph categories:
 - Baez, Fong: Passive linear circuits. $\text{PLC}: \mathcal{H} \rightarrow \mathbf{Set}$.
 - The category of relations: $\text{Rel}: \mathcal{H} \rightarrow \mathbf{Set}$.
 - Similar: The category of arrays (i.e. tensors): $\text{Arr}: \mathcal{H} \rightarrow \mathbf{Set}$.

Arrays as models $\text{Arr}: \mathcal{H} \rightarrow \text{Set}$

Setup: let k be a semi-ring. We'll consider arrays with entries in k .

- We need to add labels to the strings, namely finite sets.
 - For convenience, identify finite sets with their cardinalities in \mathbb{N} .
 - So an object $X \in \mathcal{H}$ is a finite set P and function $X: P \rightarrow \mathbb{N}$.
 - Define $\bar{X} := \prod_{p \in P} X(p)$.

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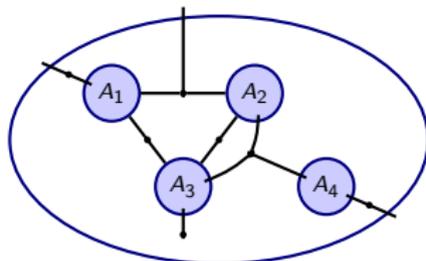
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- A cospan, as drawn below, specifies an array multiplication formula.



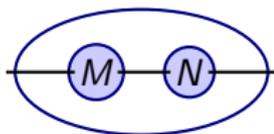
Example wiring diagrams for named operations

A single array multiplication formula returns famous matrix products.

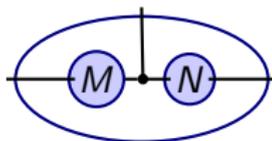
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Multiplication: MN



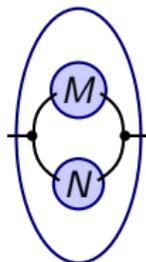
Khatri-Rao: $M \odot N$



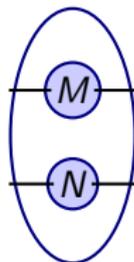
Trace: $\text{Tr}(M)$



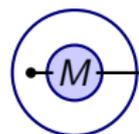
Hadamard: $M \circ N$



Kronecker: $M \otimes N$



Marginalize: $\sum_i M_{i,j}$



The real role of operads

For each type of string diagram, there is a corresponding operad \mathcal{O} .

- Operad functors allow you to change the string diagram type.
 - These generate free-forgetful adjunctions.
 - For example, the adjunction between categories and traced categories.

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 - It gives an unbiased presentation, which can be nice to have.
 - (Subjective) Engineers seem to find the perspective compelling.
 - They like the idea of building one thing out of many.
 - And they seem to understand string diagrams faster than gens/rels.

Outline

- 1 Introduction
- 2 Operads of string diagrams
- 3 Steady states are compositional**
 - Dynamical systems
 - Steady states
- 4 Conclusion

Discrete and continuous dynamical systems

Dynamical systems are machines that take input, change state, and produce output.³

- They usually come in one of two flavors: discrete and continuous.
- All of our dynamical systems are open: they can interact with others.

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Definition

A discrete (resp. continuous) dynamical system is a tuple $(S, f^{\text{upd}}, f^{\text{rdt}})$.

- S is a set (resp. manifold) of *states*;
- $f^{\text{upd}} : X^{\text{in}} \times S \rightarrow S$ (resp. $f^{\text{upd}} : X^{\text{in}} \times S \rightarrow TS$) is a function;
- $f^{\text{rdt}} : S \rightarrow X^{\text{out}}$ is function.

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Composing dynamical systems

Dynamical systems can be composed, almost like in a traced category.

- But not quite. If you allow identities, you can't have feedback.
- Related to the *traced ideals* of Abramsky, Blute, Panangaden.

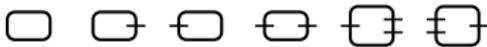
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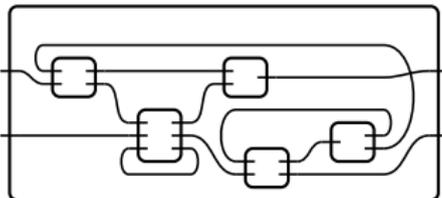
- But not quite. If you allow identities, you can't have feedback.
- Related to the *traced ideals* of Abramsky, Blute, Panangaden.
- Something like the following should be true:
 - If \mathcal{C} is a Sym.Mon.Cat, there is an operad $\mathcal{W}_{\mathcal{C}}$ such that
 - the category of traced ideals in \mathcal{C} is equivalent to $\mathbf{Fun}(\mathcal{W}_{\mathcal{C}}, \mathbf{Set})$.
 - $\mathcal{W}_{\mathcal{C}}$ is the left class of an orthogonal factorization system on $\mathbf{Cob}/\mathbf{Ob}(\mathcal{C})$.
- Dynamical systems form a traced ideal in this sense.
 - Letting \mathcal{W} be the operad $\mathcal{W}_{\mathbf{Set}}$ (resp. $\mathcal{W}_{\mathbf{Man}}$),
 - discrete (resp. continuous) dynamical systems is a model $\mathcal{W} \rightarrow \mathbf{Set}$.

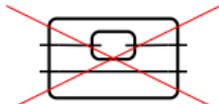
Wiring diagrams for dynamical systems

There is an operad \mathcal{W} whose objects and morphisms look like this:

objects:  etc.

morphisms:



- $\mathcal{W} \subseteq \mathit{Cob}$ is a suboperad, missing only “passing wires” 
- Think of \mathcal{W} as modeling “traced categories without identities”.

Steady states are a compositional analysis

Let \mathcal{W} be the operad of wiring diagrams as on the previous slide.

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- There is a *compositional analysis* for dynamical systems, in matrices.
 - That is, we have a model $Mat: \mathcal{W} \rightarrow \mathbf{Set}$ and
 - a natural transformation $Stst: DS \rightarrow Mat$, given by “steady states”.
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 - M 's entries are indexed by $\overline{X^{\text{in}}} \times \overline{X^{\text{out}}}$. Given $(x, y) \in \overline{X^{\text{in}}} \times \overline{X^{\text{out}}}$,
 - the *steady states* at (x, y) is $\{s \in S \mid f^{\text{upd}}(x, s) = s \text{ and } f^{\text{rdt}}(s) = y\}$.
 - $M(x, y) \in \{0, 1\}$ is 0 iff the set of steady states is empty.
 - For continuous systems, such a matrix is called the *bifurcation diagram*.

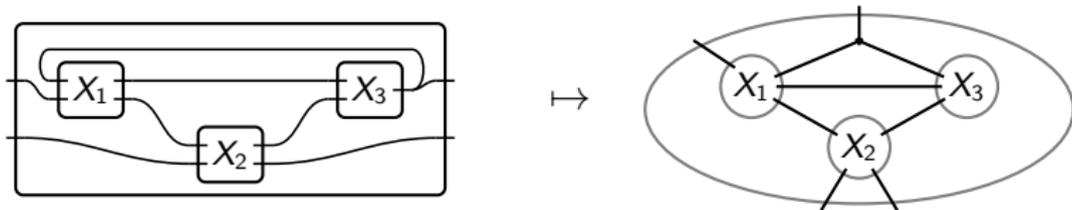
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- These steady state matrices compose according to the same \mathcal{W} .

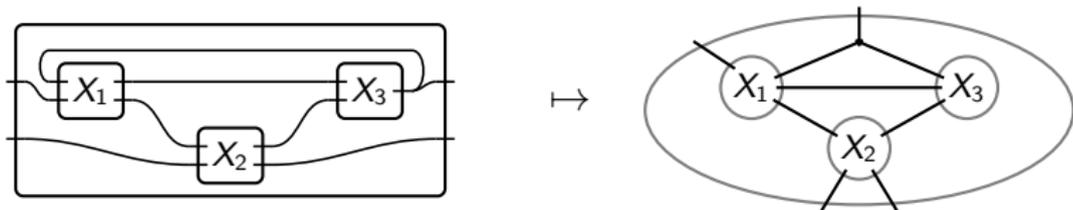
Stepping back

- Dynamical systems compose according to an operad \mathcal{W} .
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Steady states map dynamical systems to arrays via U :

$$\begin{array}{ccc}
 \mathcal{W} & \xrightarrow{U} & \mathcal{H} \\
 \searrow \text{DS} & \begin{array}{c} \text{Stst} \\ \Rightarrow \end{array} & \swarrow \text{Arr} \\
 & \text{Set} &
 \end{array}$$

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 - Compositionality vs. generative effects
 - Summary

Back to compositionality

Here's what we've been saying:

- An analysis is a way of viewing things of some type, $A: M \rightarrow N$.
- Suppose the things x can be arranged (φ 's) to create new things.
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- But what if A is merely lax, i.e. a map $N(\varphi)A(x) \rightarrow A(M(\varphi)(x))$.
 - We could call the difference a *generative effect*.
 - A is like an estimate, and the effect comes from “inexactness” of A .
 - Elie Adam (MIT) has a cohomological theory of generative effects.
 - E.g., if A is left exact, recover $A(M(\varphi))$ from cohomology of $N(\varphi)(A)$.

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Thanks for inviting me to speak!

More on steady states and the pixel array method

Discrete vs. continuous dynamical systems

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 - Then the steady state matrix is a function $\mathbb{R} \times \mathbb{R} \rightarrow \{0, 1\}$.
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 - Then the steady state matrix is a function $\mathbb{R} \times \mathbb{R} \rightarrow \{0, 1\}$.
 - This relation is usually called the *bifurcation diagram* of the DS.
- Given a wiring diagram, we must do matrix arithmetic on such beasts.
 - Calculating global steady states is tantamount to solving a system of relations.
 - This is hard in general. Generally people use Newton's method.
 - But the matrix arithmetic idea suggests another approach: pixelating.

Simple example

For simplicity, suppose we have equations $f(x, w) = 0$ and $g(w, y) = 0$.

- We plot them in some range $[-1.5, 1.5]$ using a certain pixel size.
- The plots are matrices M, N whose entries are on/off pixels.
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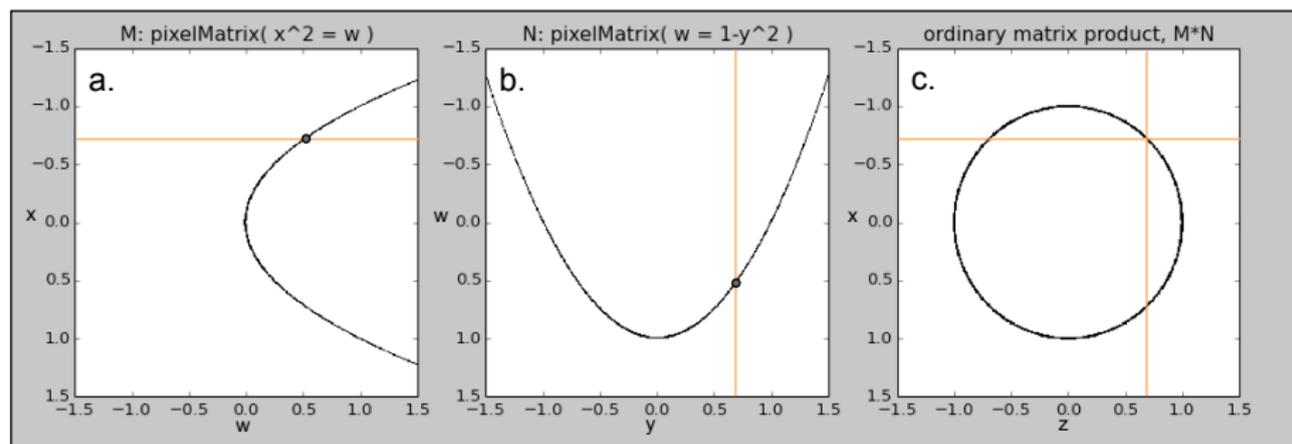
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Multiplying these two matrices MN yields the simultaneous solution.

- For example, plot equations $x^2 = w$ and $w = 1 - y^2$, and multiply.



A more complex example

Here's a more complex example:

$$\cos(\ln(z^2 + 10^{-3}x)) - x + 10^{-5}z^{-1} = 0 \quad (\text{Equation 1})$$

$$\cosh(w + 10^{-3}y) + y + 10^{-4}w = 2 \quad (\text{Equation 2})$$

$$\tan(x + y)(x - 2)^{-1}(x + 3)^{-1}y^{-2} = 1 \quad (\text{Equation 3})$$

Q: For what values of w and z does a simultaneous solution exist?⁴

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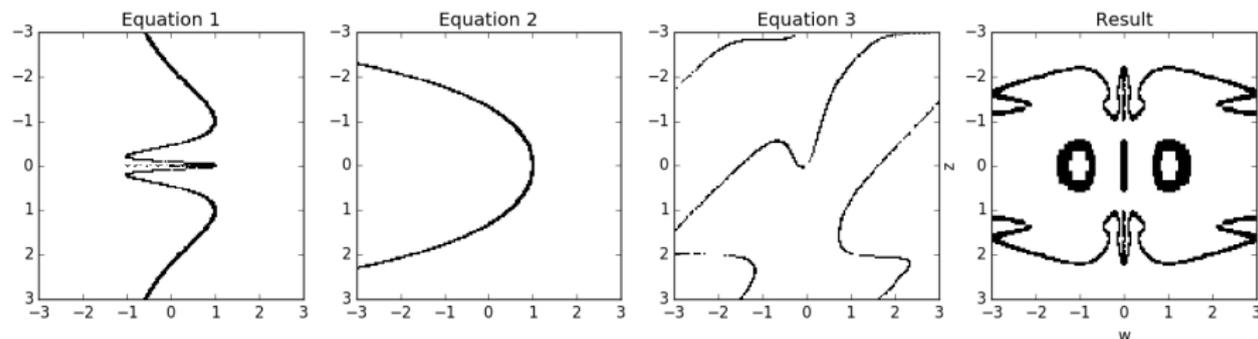
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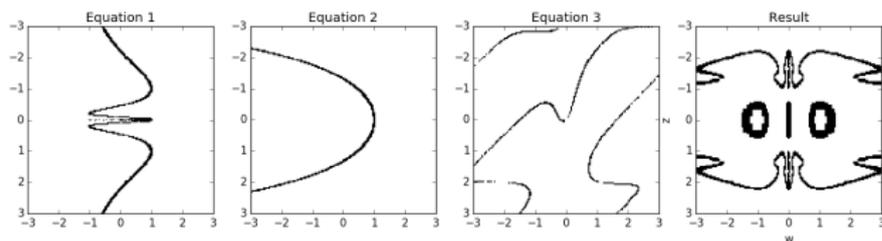


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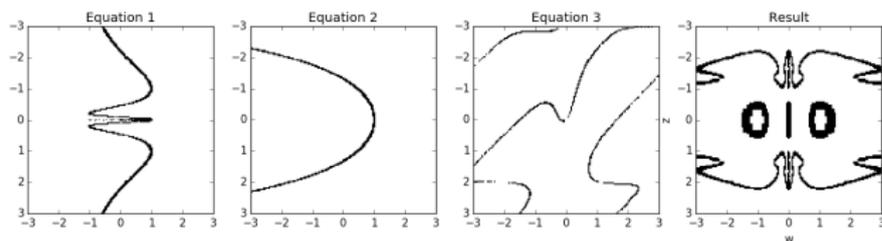
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- Upshot: we can actually find steady states of systems of systems.
 - For discrete dynamical systems, it works on the nose.
 - For continuous ones, we use pixel arrays.
 - It's an estimate, but it converges and we can bound the error.