An Operadic Approach to Compositionality

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Outline

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- This leads naturally to the notion of operad $\mathcal{O}$, which specifies:
  - the set of possible things $X, Y, \ldots$;
  - the set of arrangements φ, ψ by which one thing is composed of many;
  - how nesting works $\psi \circ (\varphi_1, \ldots, \varphi_n)$.

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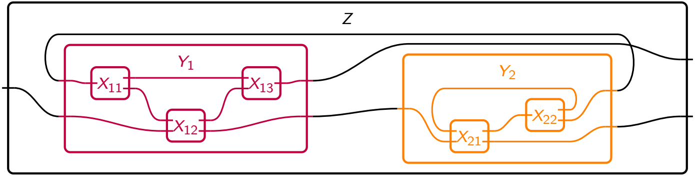
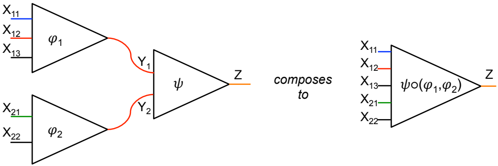
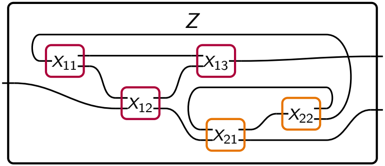
- Note: by *operad*, I mean what is usually called "colored operad".

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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Syntax and semantics

- An operad $\mathcal{O}$ specifies a *theory of composition*.
  - $\mathcal{O}$ specifies various kinds of things and how they can be arranged.
  - These are the sorts and the operations in our theory $\mathcal{O}$ of composition.
- Functorial semantics: a *model of* $\mathcal{O}$ is a functor $M\colon \mathcal{O} \to \mathbf{Set}$.
  - For every sort $X \in \mathcal{O}$, we have a set $M(X)$ of things of that sort.
  - For every arrangement $\varphi\colon X_1, \ldots, X_n \to Y$ in $\mathcal{O}$, we have a function
  $$M(\varphi)\colon M(X_1) \times \cdots \times M(X_n) \to M(Y).$$
    - Given a tuple $(x_1, \ldots, x_n) \in M(X_1) \times \cdots \times M(X_n)$,
    - and a rule φ for assembling them,
    - we obtain some new $\varphi(x_1, \ldots, x_n) \in M(Y)$.
- 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 $M\colon \mathcal{O} \to \mathbf{Set}$.
  - 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 $A\colon M \to N$.
  - To each sort $X \in \mathcal{O}$, we have an attribute $A_X\colon M(X) \to N(X)$.

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  - To each sort $X \in \mathcal{O}$, we have an attribute $A_X\colon M(X) \to N(X)$.
  - *Compositionality*: for any arrangement φ and things $x_1, \ldots, x_n$, we have

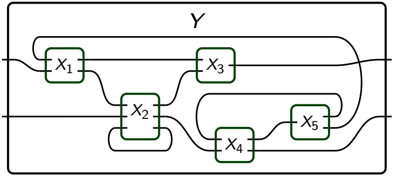
$$A_Y\big(M(\varphi)(x_1, \ldots, x_n)\big) = N(\varphi)\big(A_{X_1}(x_1) \ldots, A_{X_n}(x_n)\big)$$

- 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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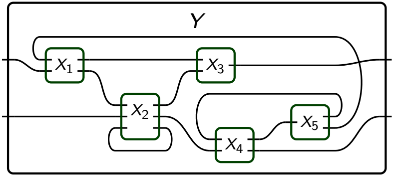

- We'll discuss a model $\mathrm{DS}\colon \mathcal{W} \to \mathbf{Set}$ of "dynamical systems".
- There is a compositional analysis $A\colon \mathrm{DS} \to \mathrm{Mat}$.
  - Here, $\mathrm{Mat}\colon \mathcal{W} \to \mathbf{Set}$ is the model of matrices.
  - A assigns to each dynamical system its 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, $\mathrm{Prot}\colon \mathcal{M} \to \mathbf{Set}$.[1]

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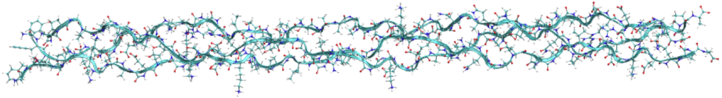
- A new protein can be assembled from a finite set of proteins
  - arranged in series or parallel, or
  - arranged in helices, double helices, any conceivable curve, etc.



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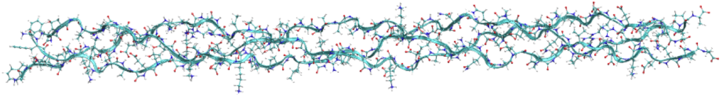

- A compositional analysis would be "incredibly" useful in mat. sci.:
  - Example: assign a value, e.g. strength or toughness, to each protein
  - with a formula for composing strengths according to any arrangement.
  - Even if not perfectly compositional, it would be highly valuable.

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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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  - They give us a visual tool for solving algebra problems.
  - Peter Selinger's survey of graphical languages is fun and helpful.

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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 $M\colon \mathcal{O} \to \mathbf{Set}$.

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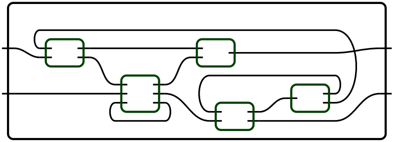
  - The connection between string diagrams and their meaning is a functor $M\colon \mathcal{O} \to \mathbf{Set}$.
- Below is an example string diagram for traced monoidal categories.

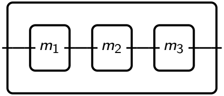


- We want to encode such diagrams as mathematical objects.

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 T is (as always) a functor $M\colon \mathcal{T} \to \mathbf{Set}$.
  - It assigns to the unique object $*$ a set $M := M(*)$.
  - It assigns an operation $M^n = M \times \cdots \times M \to M$ for every n.



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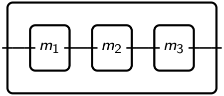

  - The composition formula in $\mathcal{T}$ ensures the associativity and unitality.
- One can think of this as an "unbiased" perspective on monoids:
  - $\mathcal{T}$ gives us all the operations (n-ary multiplication) on equal footing,
  - in contrast to the usual approach: two generators, unit and mult.

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.
  - I'd like a nice way to deal with this, but haven't settled on anything.

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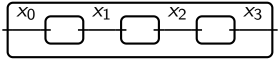
  - I'd like a nice way to deal with this, but haven't settled on anything.
- Choose Λ. Define $\mathcal{O}_\Lambda$ as the following operad.
  - Its objects are pairs $X = (x_1, x_2) \in \Lambda^2$, drawn x_1  x_2.
  - Its n-ary morphisms $X_1, \ldots, X_n \to Y$ are tuples $(x_0, \ldots, x_n) \in \Lambda^{n+1}$,
  - ... such that $X_i = (x_{i-1}, x_i)$ and $Y = (x_0, x_n)$.



- A model $\mathcal{C} \colon \mathcal{O}_\Lambda \to \mathbf{Set}$ 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 $\mathcal{C}ob$

Modulo string labels, the operad for traced monoidal categories is $\mathcal{C}ob$:[2]

Theorem

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

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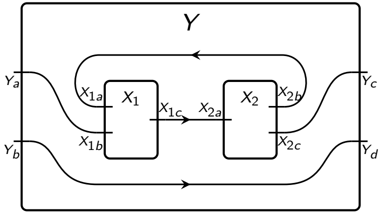

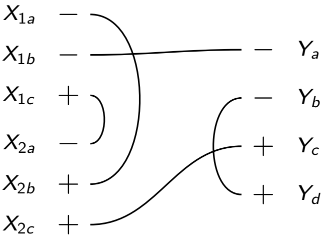

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Hypergraph categories

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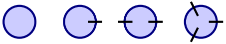
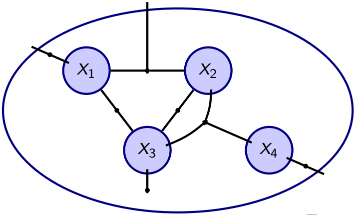
But the concept is quite easy from the perspective of string diagrams.

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

objects:  etc.

morphisms: 

Operad $\mathcal{H} = \mathcal{C}ospan$ 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 $\mathcal{H} = \mathcal{C}ospan$.
  - If no, then $\mathcal{H} = \mathcal{C}orel$. (This is the definition I used above; see Fong.)

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- Either way, objects are finite sets (the set of ports) 
  - Morphisms are either cospans $X_1 \sqcup \cdots \sqcup X_n \to L \leftarrow Y$
  - or jointly surjective cospans $X_1 \sqcup \cdots \sqcup X_n \sqcup Y \twoheadrightarrow L$.

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  - or jointly surjective cospans $X_1 \sqcup \cdots \sqcup X_n \sqcup Y \twoheadrightarrow L$.
- Examples of hypergraph categories:
  - Baez, Fong: Passive linear circuits. $\mathrm{PLC}\colon \mathcal{H} \to \mathbf{Set}$.
  - The category of relations: $\mathrm{Rel}\colon \mathcal{H} \to \mathbf{Set}$.
  - Similar: The category of arrays (i.e. tensors): $\mathrm{Arr}\colon \mathcal{H} \to \mathbf{Set}$.

Arrays as models $\mathrm{Arr}\colon \mathcal{H} \to \mathbf{Set}$

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 $X\colon P \to \mathbb{N}$.
  - Define $\overline{X} := \prod_{p \in P} X(p)$.

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- To each X we assign the set $\mathrm{Arr}(X) := \{A\colon \overline{X} \to k\}$.
  - So if $P = 1, 2$ and $X(1) = m$ and $X(2) = n$ then
  - $\overline{X} = m \times n$ and $\mathrm{Arr}(X)$ is the set of $m \times n$ matrices.

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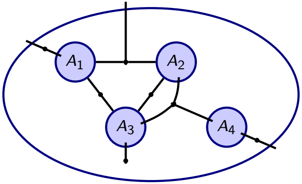
  - $\overline{X} = m \times n$ and $\mathrm{Arr}(X)$ is the set of $m \times n$ matrices.
- A cospan, as drawn below, specifies an array multiplication formula.



Example wiring diagrams for named operations

A single array multiplication formula returns famous matrix products.

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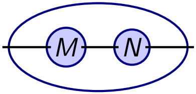
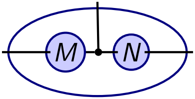
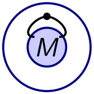
Multiplication: MN



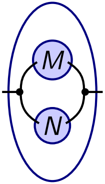
Khatri-Rao: $M \odot N$



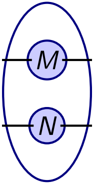
Trace: $\mathrm{Tr}(M)$



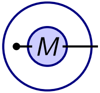
Hadamard: $M \circ N$



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 $\mathcal{O}$.

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- Operad functors allow you to change the string diagram type.
  - These generate free-forgetful adjunctions.
  - For example, the adjunction between categories and traced categories.
- Working directly with doctrines is often preferable to using operads.
  - People understand faster w/o operads. (Traced cat vs. $\mathcal{C}ob$-model).
  - You don't have to worry about object labels.

The real role of operads

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- Operad functors allow you to change the string diagram type.
  - These generate free-forgetful adjunctions.
  - For example, the adjunction between categories and traced categories.
- Working directly with doctrines is often preferable to using operads.
  - People understand faster w/o operads. (Traced cat vs. $\mathcal{C}ob$-model).
  - You don't have to worry about object labels.
- On the other hand, there are sometimes reasons to prefer operads:
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    - E.g. traced cats without identities are perfect for dynamical systems.
    - String diagrams may be more basic than their generators and relations.

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    - E.g. traced cats without identities are perfect for dynamical systems.
    - String diagrams may be more basic than their generators and relations.
  - 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

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*;
- $f^{\text{upd}}\colon X^{\text{in}} \times S \to S$ (resp. $f^{\text{upd}}\colon X^{\text{in}} \times S \to TS$) is a function;
- $f^{\text{rdt}}\colon S \to X^{\text{out}}$ is function.

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Composing dynamical systems

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

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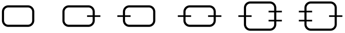
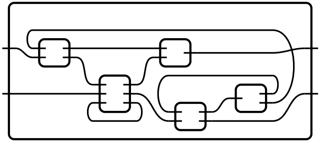
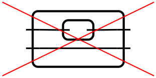
- But not quite. If you allow identities, you can't have feedback.
- Related to the *traced ideals* of Abramsky, Blute, Panangaden.
- Something like the following should be true:
  - If $\mathcal{C}$ is a Sym.Mon.Cat, there is an operad $\mathcal{W}_{\mathcal{C}}$ such that
  - the category of traced 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 $\mathcal{C}ob_{/\mathrm{Ob}(\mathcal{C})}$.
- 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 $\mathcal{W} \to \mathbf{Set}$.

Wiring diagrams for dynamical systems

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

objects:  etc.

morphisms: 

- $\mathcal{W} \subseteq \mathcal{C}ob$ 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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  - That is, we have a model $\mathrm{Mat}\colon \mathcal{W} \to \mathbf{Set}$ and
  - a natural transformation $\mathsf{Stst}\colon \mathrm{DS} \to \mathrm{Mat}$, given by "steady states".
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  - Let $F = (S, f^{\mathrm{upd}}, f^{\mathrm{rdt}})$ be the dynamical system and $M := \mathsf{Stst}(F)$.
  - M's entries are indexed by $\overline{X^{\mathrm{in}}} \times \overline{X^{\mathrm{out}}}$. Given $(x, y) \in \overline{X^{\mathrm{in}}} \times \overline{X^{\mathrm{out}}}$,
    - the *steady states* at (x, y) is $\{s \in S \mid f^{\mathrm{upd}}(x, s) = s \text{ and } f^{\mathrm{rdt}}(s) = y\}$.
    - $M(x, y) \in \{0, 1\}$ is 0 iff the set of steady states is empty.
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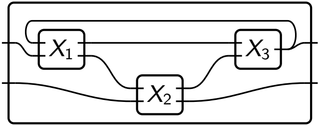
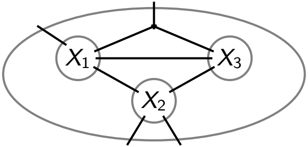
- These steady state matrices compose according to the same $\mathcal{W}$.

Stepping back

- Dynamical systems compose according to an operad $\mathcal{W}$.
- Arrays compose according to an operad $\mathcal{H}$.
- There's an operad functor $U\colon \mathcal{W} \to \mathcal{H}$.



$\mapsto$



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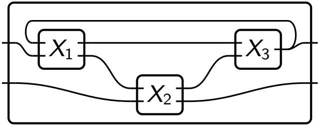

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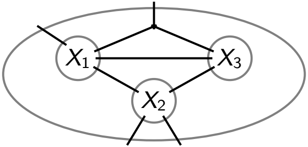

Steady states map dynamical systems to arrays via U:

$$
\begin{tikzcd}
\mathcal{W} \arrow[rr, "U"] \arrow[dr, "\mathrm{DS}"'] \arrow[rr, phantom, shift right=5, "\overset{\mathsf{Stst}}{\Rightarrow}"] & & \mathcal{H} \arrow[dl, "\mathrm{Arr}"] \\
& \mathbf{Set} &
\end{tikzcd}
$$

Outline

Back to compositionality

Here's what we've been saying:

- An analysis is a way of viewing things of some type, $A\colon M \to N$.
- Suppose the things x can be arranged (φ's) to create new things.
  - The analysis A is compositional if it commutes with φ's.
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  - That is, there is an isomorphism $N(\varphi)A(x) \cong A(M(\varphi)(x))$
- But what if A is merely lax, i.e. a map $N(\varphi)A(x) \to A(M(\varphi)(x))$.
  - 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 $N(\varphi)(A)$.

Summary

In this talk, we discussed the following:

- A general definition of composition and compositionality.
  - Composition is building one thing out of many.
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  - How it'd be nice to have compositional analyses of materials.

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  - How it'd be nice to have compositional analyses of materials.
- Operads describe string diagrams of known categorical doctrines.
  - Monoids and categories: basically the terminal operad, plus labels.
  - Traced monoidal categories: the operad *Cob* of oriented cobordisms.
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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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  - 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.
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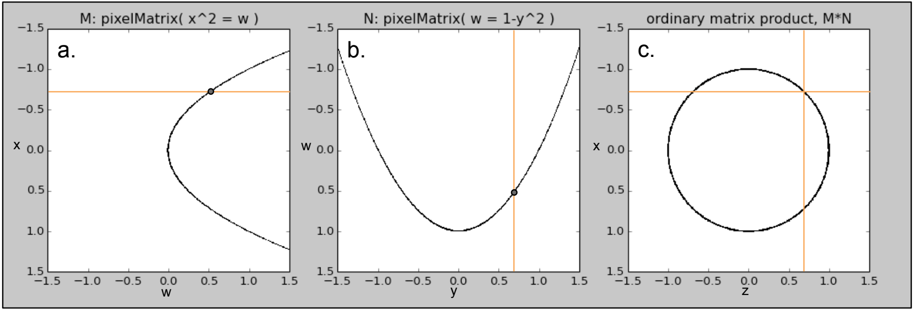
Multiplying these two matrices MN yields the simultaneous solution.

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



A more complex example

Here's a more complex example:

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

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

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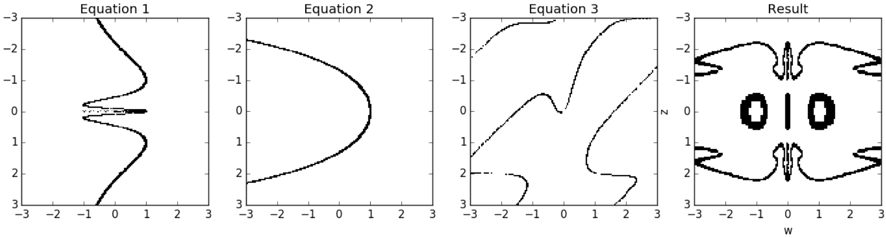

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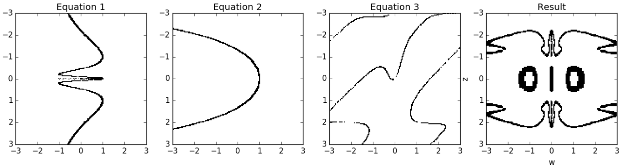
Pixel array method

I call this the *pixel array method*.

- We can solve systems by plotting and multiplying arrays.
- This gives good results, both in terms of speed and accuracy.
  - We also see the whole solution set, which could be quite useful.



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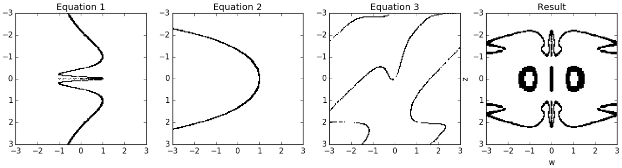

- Upshot: we can actually find steady states of systems of systems.
  - For discrete dynamical systems, it works on the nose.
  - For continuous ones, we use pixel arrays.
  - It's an estimate, but it converges and we can bound the error.