

Some Applications of Category Theory

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The need for organizational frameworks

Consider: “organizational frameworks for thinking”

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 - Arithmetic, algebra, calculus, probability
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- New math can be invented for thinking about today's world:
 - Frameworks for thinking about multi-level systems
 - Ways of translating information from one field to another
 - I propose that category theory can work well for this.

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- What about outside of math?

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Why? What does it really do?

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 - In CS, programs are relationships between datatypes
 - (Higher level): Java can be compiled to machine code
- Like a symphony, complex things are composed from simpler pieces.
 - Relationships between notes, relationships between instruments
 - CT gives a very general notion of composition.
 - “Composition” is the subject of the talk.

Plan of the talk

I'll discuss CT as mathematics for organizing thought.

- Main thrust: “composition”, putting things together
- Formal notion: *operads*, a general framework for composition
 - I'll give examples and sketch a definition.
 - Operads: the mathematical framework for the talk

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A lot of information coming: try to get the overarching storyline.

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An operad consists of:

- A collection of **objects** X, Y, \dots ,
- And ways to **arrange** them, $\varphi: X_1, \dots, X_k \rightarrow Y$,
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Slightly more formal definition to come.

Operads are everywhere

Operads are used unconsciously in many fields.

- Electrical engineering: “wiring diagrams”.
- Design: “set-based design”.
- Computer programming: “data flow”.
- Natural language processing: “grammars”.
- Materials science: “hierarchical materials”.

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Rallying cry: *Let's bring operads to the fore.*

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- Operads structure and organize this sort of thinking.
- With mathematical structure, we can go much further.

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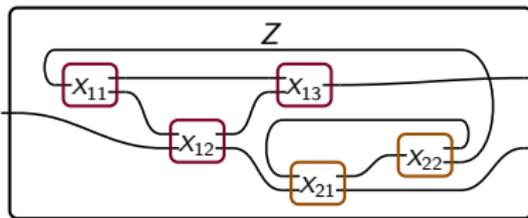
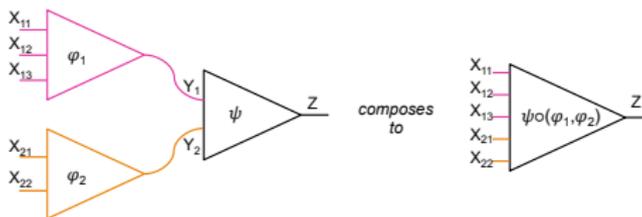
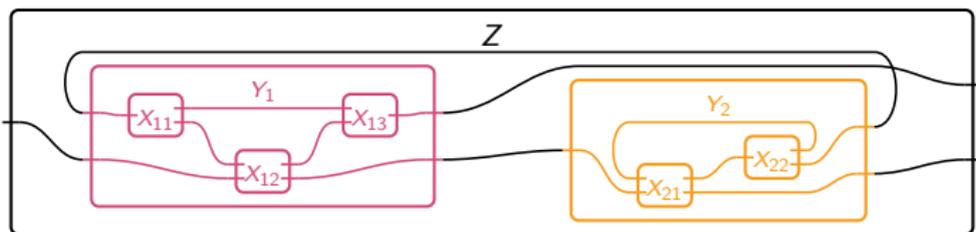
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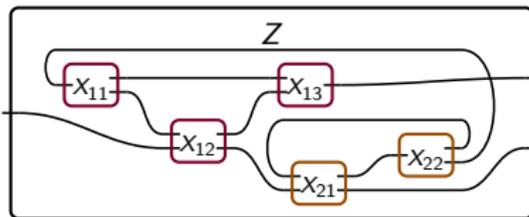
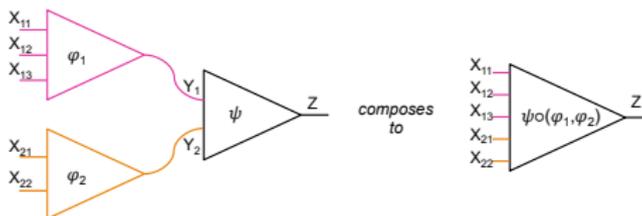
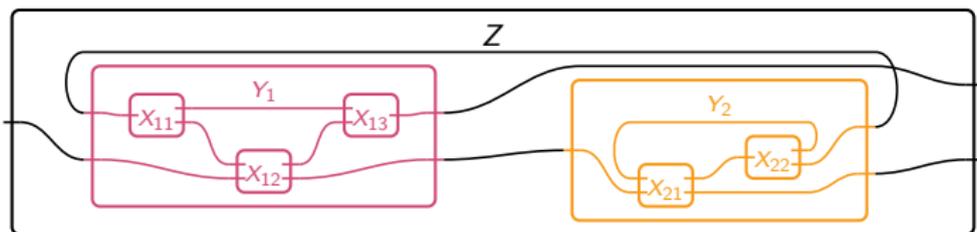
Let's look for **objects**, **arrangements**, and **nesting** in some examples.

Operad 1: wiring diagrams



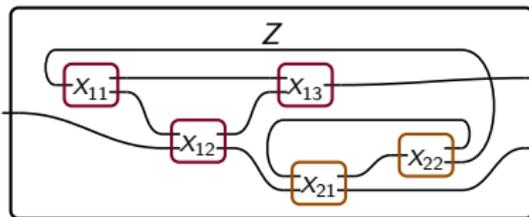
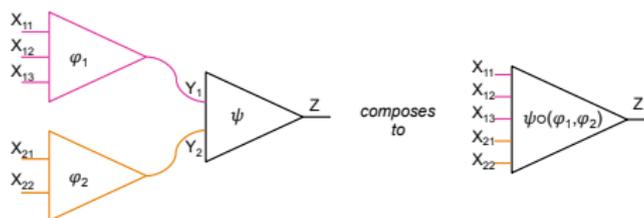
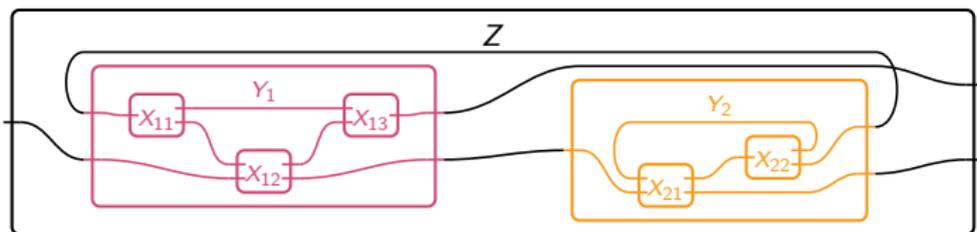
Objects: boxes with ports.

Operad 1: wiring diagrams



Objects: boxes with ports. Arrangements: wiring diagrams.

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Objects: boxes with ports. Arrangements: wiring diagrams. Nesting: nesting.

Formal definition of operad

An operad \mathcal{O} consists of

- A set $\text{Ob}(\mathcal{O})$, elements of which are called *objects*.
- For objects $X_1, \dots, X_k, Y \in \text{Ob}(\mathcal{O})$, a set

$$\text{Mor}_{\mathcal{O}}(X_1, \dots, X_k; Y)$$

Its elements are called *morphisms* or **arrangements** of X_1, \dots, X_k in Y .
An arrangement $\varphi \in \text{Mor}_{\mathcal{O}}(X_1, \dots, X_k; Y)$ may be denoted

$$\varphi: X_1, \dots, X_k \rightarrow Y.$$

- For each object $X \in \text{Ob}(\mathcal{O})$, an identity arrangement $\text{id}_X: (X) \rightarrow X$.
- A composition, or **nesting** formula, e.g.,

$$\psi \circ (\varphi_1, \dots, \varphi_k): (X_{i,j}) \xrightarrow{\varphi_i} (Y_i) \xrightarrow{\psi} Z.$$

These are required to satisfy well-known “unital” and “associative” laws.

Operad 1: WDs again

An operad \mathcal{W} for composing wiring diagrams:

- **Object** $X \in \mathcal{W}$: any possible box-with-ports.



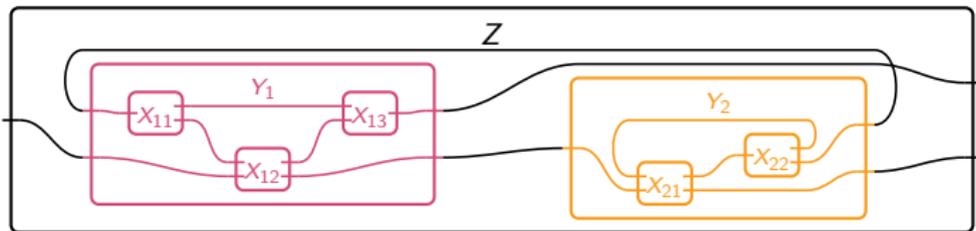
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An operad \mathcal{W} for composing wiring diagrams:

- **Object** $X \in \mathcal{W}$: any possible box-with-ports.



- **Arrangement** $\phi: X_1, \dots, X_k \rightarrow Y$ in \mathcal{W} : any wiring of X 's in Y .
- **Nesting**: the facts about how wiring diagrams fit inside each other.



One operad \mathcal{W} comprises all this.

Operad 2: hierarchical protein materials

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

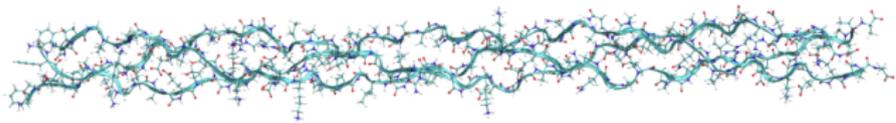
- A **protein** is an **arrangement** of simpler **proteins**.
 - There are “atomic” proteins: amino acids.
 - Protein materials include your skin: stretchable, breathable, waterproof.
 - Materials scientists would *love* to make materials like this.

¹Giesa, T.; Jagadeesan, R.; Spivak, D.I.; Buehler, M.J. (2015) “Matriarch: a Python library for materials architecture.” *ACS Biomaterials Science & Engineering*.

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 - Materials scientists would *love* to make materials like this.
- **Assemble** new **proteins** from old:
 - arrange in series or parallel (H-bonds), or
 - arrange in helices, double helices, any conceivable curve, etc.



- Collagen has a **nested** structure: it is an array, each fiber of which is a triple helix, each strand of which is a helix, each unit of which is an amino acid.¹

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More operads: Grammars and recipes

Context-free grammars are “free” operads.

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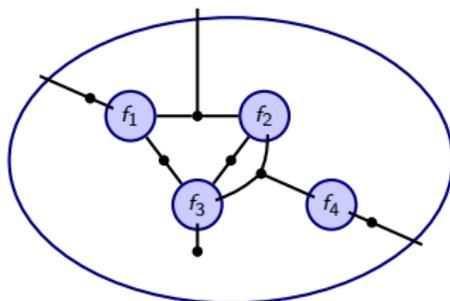
Recipes are also operads.

- Combine sub-recipes to make a recipe.
- The outline for this talk as an operad:
 - **Objects**: points I want to make.
 - **Arrangements**: putting points together to make a bigger point.
 - **Nesting**: the well-known outline structure.

Grammars and recipes organize communication and action.

Quickly: an operad we'll see later

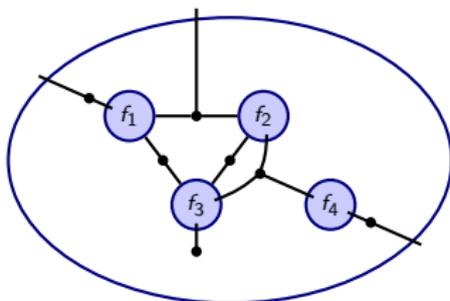
Another sort of wiring diagram (WD):



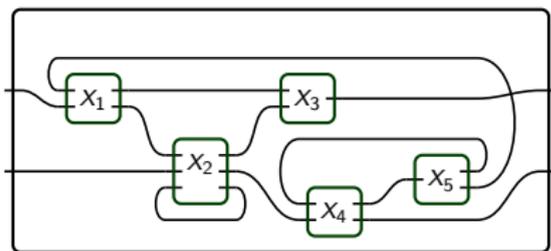
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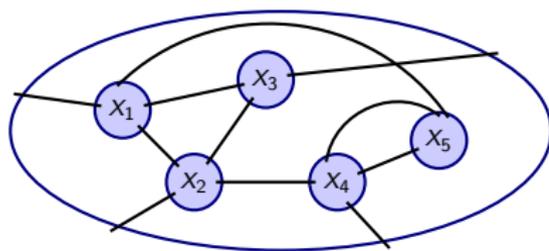
Another sort of wiring diagram (WD):



- This operad is an unoriented version of the first.
- Any oriented WD can be converted to an unoriented one.



\rightsquigarrow



Operads and their algebras

One more formal notion to discuss: algebras.

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Operad = theory. Algebras = models.

Each operad has many algebras

Each operad \mathcal{O} is a “theory of composition”.

- **Objects** X, Y, \dots : what *sorts* of elements in this theory?
- **Arrangements** ϕ, ψ : what are the operations?
- **Nesting**: what kind of laws?

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The \mathcal{O} -algebras are the models of theory \mathcal{O} .²

- An \mathcal{O} -algebra A says what’s actually being composed.
 - To each **object** X : a set $A(X)$ of elements.
 - To each **arrangement** ϕ : an k -ary operation $A(\phi)$.
 - If $\phi: X_1, \dots, X_k \rightarrow Y$ is an arrangement,
 - Then $A(\phi): A(X_1) \times \dots \times A(X_k) \rightarrow A(Y)$ is a function.
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Next, I’ll explain what algebras on an operad look like.

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Example: the operad for monoids

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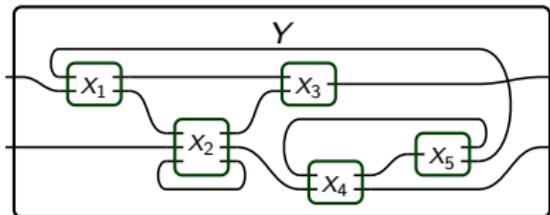
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- The operad laws (unitality, associativity) guarantee the monoid laws.

Takeaway: The simplest operad is the one for monoids.

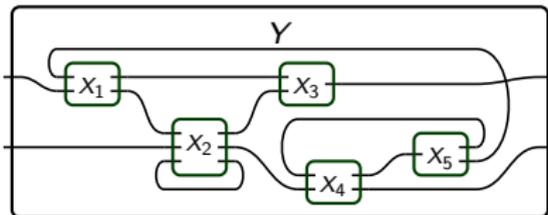
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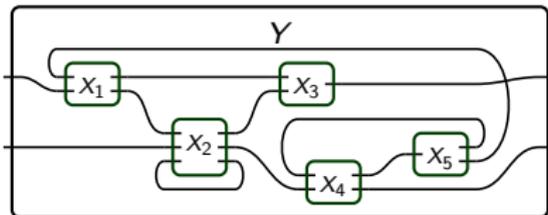


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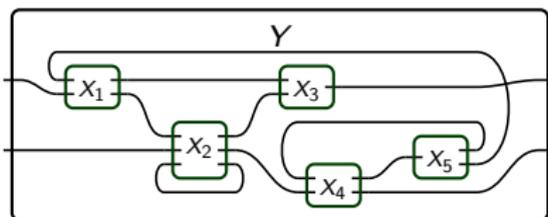


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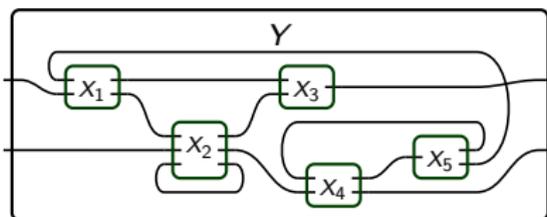


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We'll see next that “open dynamical systems” form an algebra.

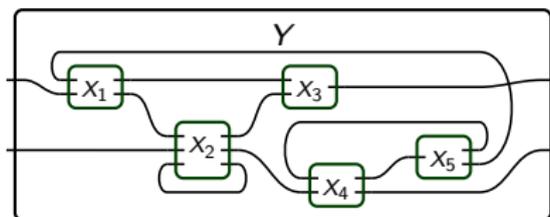
\mathcal{W} -algebra 1: open dynamical systems (ODS's)



To each box X : open dynamical systems = machines with ports.

- Let k and ℓ be the number of input and output wires on X .
- X is assigned a state space, \mathbb{R}^n .

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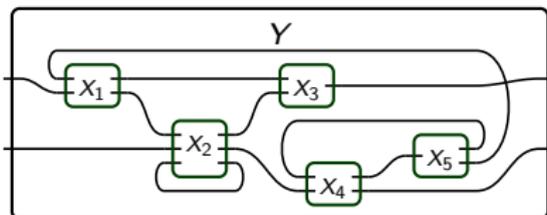
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- X is assigned a system of ordinary differential equations:

$$\begin{array}{ll}
 \dot{x}_1 = f_1(x_1, \dots, x_n, a_1, \dots, a_k) & b_1 = g_1(x_1, \dots, x_n) \\
 \dot{x}_2 = f_2(x_1, \dots, x_n, a_1, \dots, a_k) & b_2 = g_2(x_1, \dots, x_n) \\
 \vdots = \vdots & \vdots = \vdots \\
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 \end{array}$$

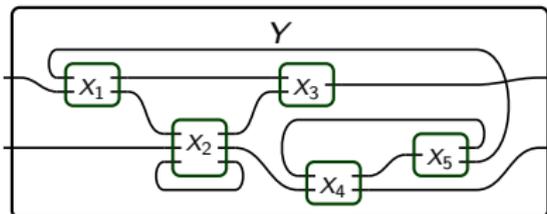
Continuously: change state based on current state and input; send output.

\mathcal{W} -algebra 1: open dynamical systems (ODS's)



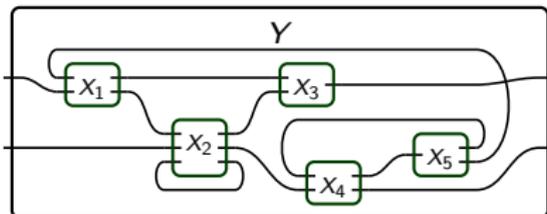
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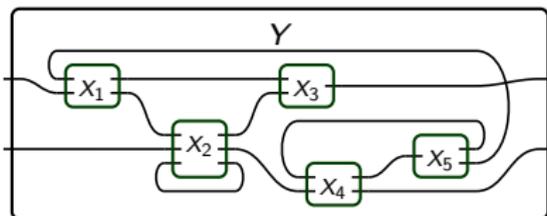
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Operad and algebra: organize thinking about composing dynamical systems.

Flavors of dynamical systems, as \mathcal{W} -algebras

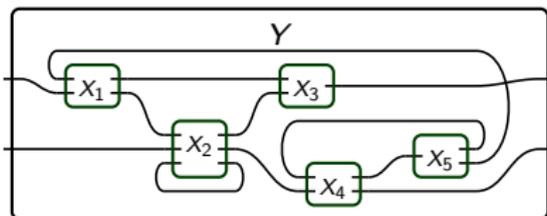


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- A_1 : continuous ODS's (ODE's with time-varying parameters).³

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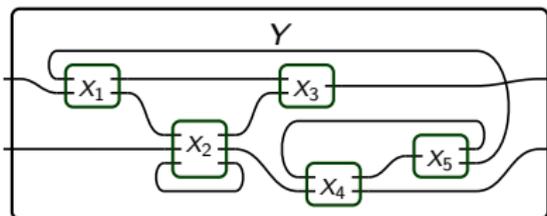
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But there are somewhat different-seeming algebras too.

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What's a relation?

Relations are everywhere.

- Definition: $R \subseteq A_1 \times A_2 \times \cdots \times A_n$.
 - Here R is “an n -ary relation on A_1, \dots, A_n ”.
 - Out of all the tuples (a_1, \dots, a_n) , R tells us which are “related”.
 - We can write R as $\{(a_1, \dots, a_n) \in A_1 \times \cdots \times A_n \mid \text{property } R\}$.

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- Relations are the foundation of database theory. Examples:
 - $\{(p, c) \in \text{Person} \times \text{Person} \mid p \text{ is a parent of } c\}$
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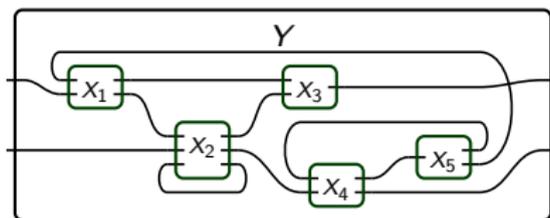
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- They're also subsets of Euclidean spaces:
 - $\{(x, y) \in \mathbb{R} \times \mathbb{R} \mid x^2 + y^2 = 1\}$.
 - $\{x \in \mathbb{R} \mid x \geq 5\}$.

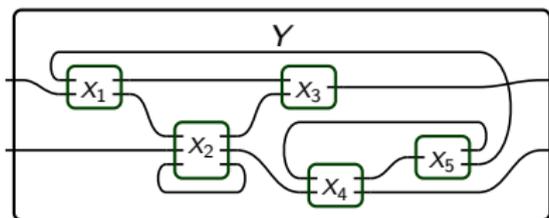
Relations are not dynamic at all, but they still form a \mathcal{W} -algebra.

Relations are a \mathcal{W} -algebra



Imagine the ports/wires are labeled with sets.

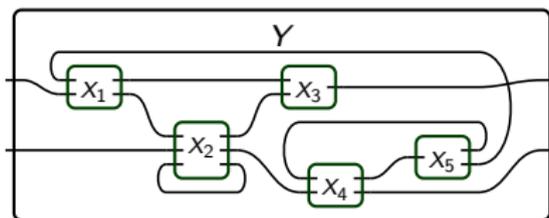
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More on this later. First, let's discuss tensors.

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Matrix: 2-dimensional array; Tensor: n -dimensional analogue.

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- For example, consider a $(2 \times 5 \times 2 \times 3)$ -tensor T .
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- Operations on tensors: Kronecker and contraction.
 - Given tensors $T: d_1 \times d_2$ and $U: d_3 \times d_4 \times d_5$.
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 - Contract: can do it if any two dimensions match, say $d_1 = d_4$.
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 - Like matrix multiplication, result is $d_2 \times d_3 \times d_5$:

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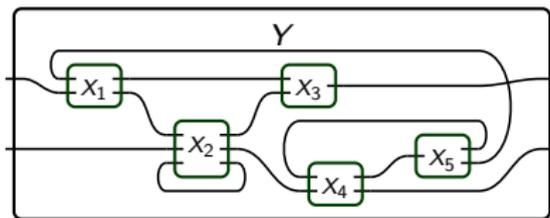
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$$V(i_2, i_3, i_5) = \sum_{j=1}^d T(j, i_2) * U(i_3, j, i_5)$$

Tensors are a \mathcal{W} -algebra

Tensors are not dynamic at all, but they still form a \mathcal{W} -algebra.

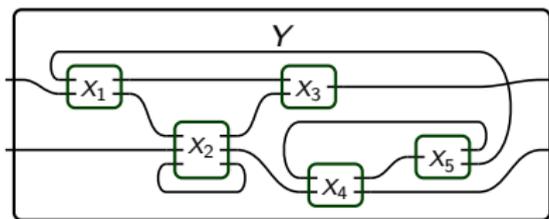


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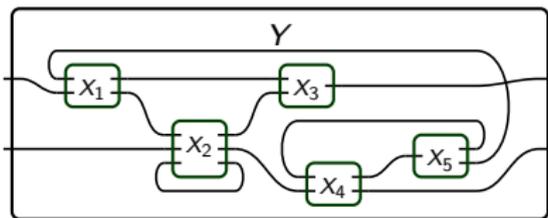


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Next up: using this algebra for solving general systems of equations.

Detailed look at an application

Separately plot the solutions to equations: $f(x, w) = 0$ and $g(w, y) = 0$.

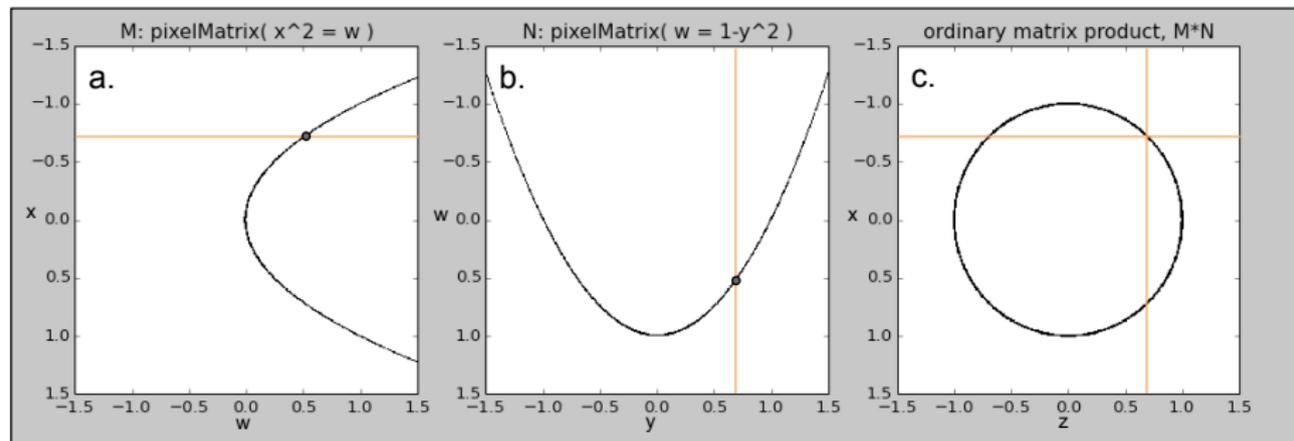
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Example: $x^2 = w$ and $w = 1 - y^2$.



A more complex example

The following eq's are not differentiable, nor even defined everywhere.

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

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

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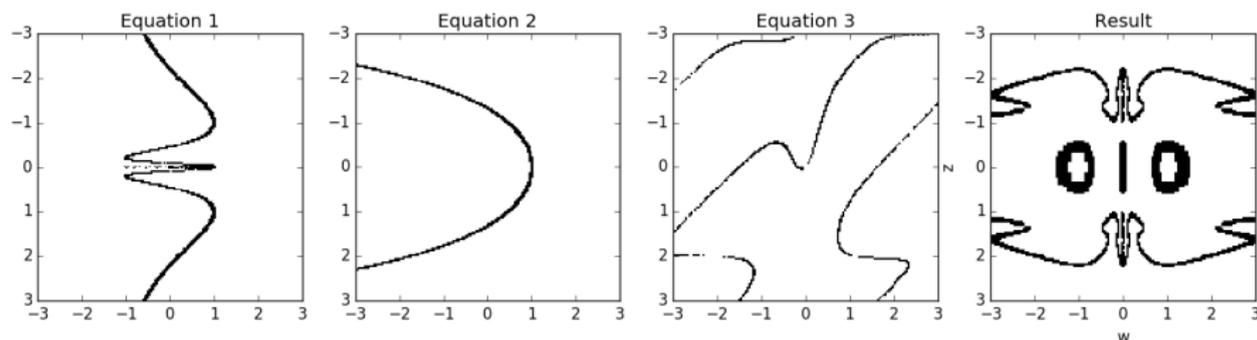
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Equations and wiring diagrams

Consider an arbitrary system of equations having the following form:

$$f_1(\mathbf{t}, u, \mathbf{v}) = 0$$

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$$f_4(x, \mathbf{z}) = 0$$

Bold variables are those we want to *expose*; others are *unexposed*.

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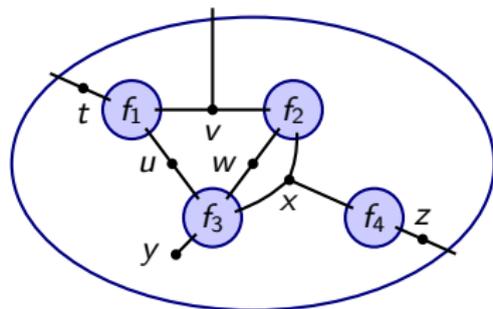
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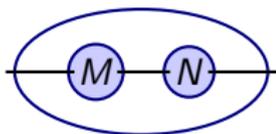


Said another way, we want $\{(t, v, z) \mid \exists u, w, x, y : f_1 = f_2 = f_3 = f_4 = 0\}$.

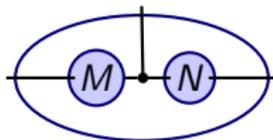
Example wiring diagrams for named operations

Some famous matrix products as wiring diagrams:

Multiplication: MN



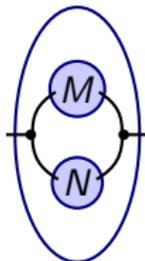
Khatri-Rao: $M \odot N$



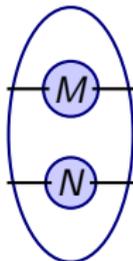
Trace: $\text{Tr}(M)$



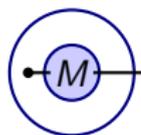
Hadamard: $M \circ N$



Kronecker: $M \otimes N$

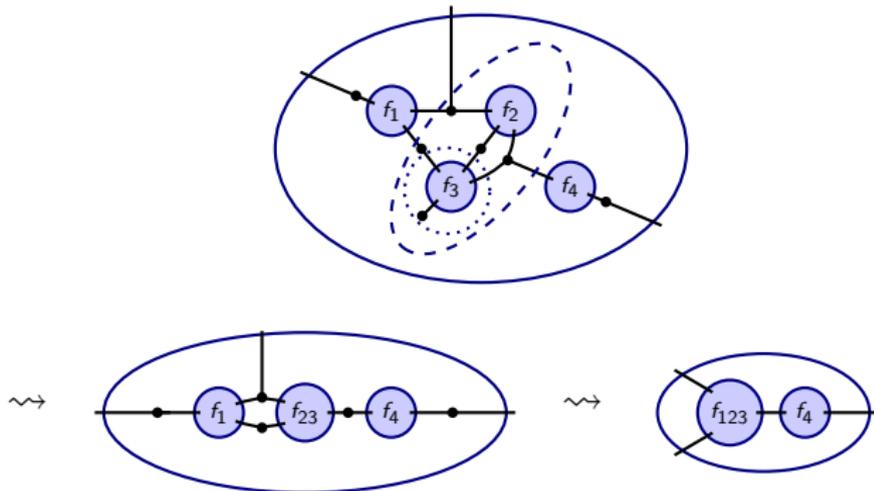


Marginalize: $\sum_i M_{i,j}$



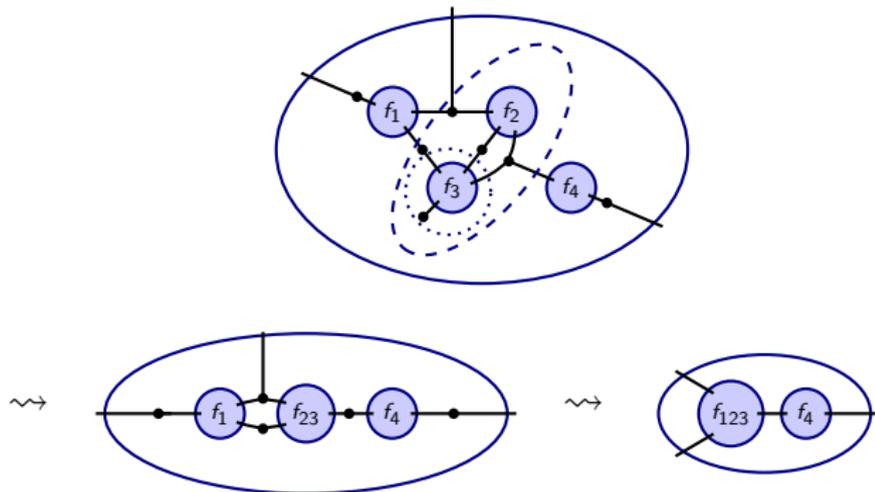
Clustering for speed

To solve systems of equations fast, cluster:



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The operad associative law lets you choose the order.

- Order of contracting edges doesn't affect solution.
- But it does affect speed.

Speed test: apples and oranges

The inputs and outputs of the PA method are different than Newton's.

	Pixel Array method	Newton's method
Inputs:	a range for each variable	a good initial guess
Outputs:	all solutions for some variables	one solution in all variables.

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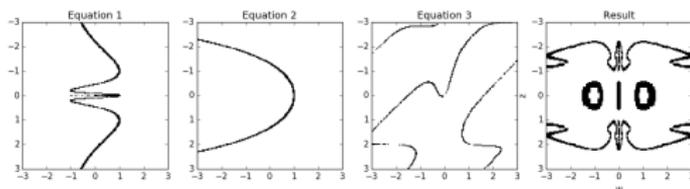
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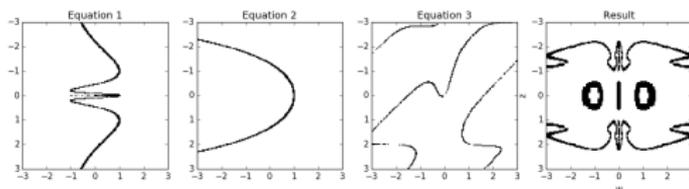
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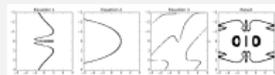


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Above case: PA was over 7200x faster.

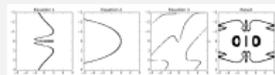
- PA: 1.5 seconds; Newton: we stopped Julia's NLSolve after 3 hours.
- PA was faster in every partially-decomposable system we tried.

Accuracy of the pixel array method



Output accuracy = input accuracy.

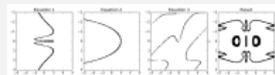
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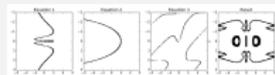
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- PA method: multiply plots as tensors.
- Result (solution) has the same guarantees:
 - If there is a solution in a pixel, it is marked.
 - If a pixel is marked, then the pixel is 2ϵ -close to a solution.

Where we are

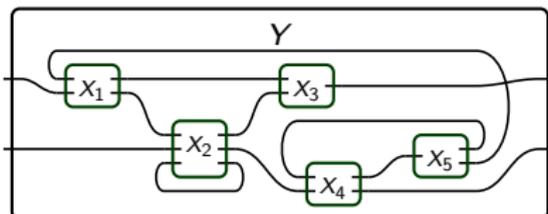
The talk is almost done!

- Discussed operads: general compositional structures
- Lots of algebras on the wiring diagrams operad \mathcal{W}
 - Open dynamical systems: behavior of interacting machines
 - Relations: find simultaneous solutions
 - Tensors: contract tensor networks
- Discussed the pixel array method
 - It turns relations into tensors by plotting.
 - Plotting is “compositional”: solve-then-plot = plot-then-contract

Last thing: discuss compositional mappings for dynamical systems.

Compositional mappings

Suppose there's a continuous DS in each box:



Two choices; what's the difference?

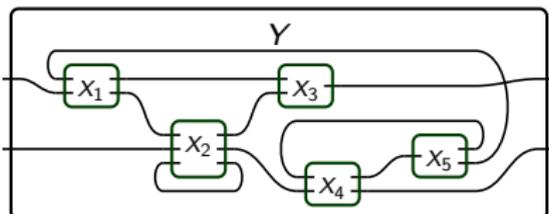
- Choice 1: compose the continuous systems and discretize the result;
- Choice 2: discretize each and then compose the discrete systems.

⁵Spivak "The steady states of dynamical systems". *arXiv* 1512.00802.

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Compositional mappings

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“Discretization is compositional”: you get the same result either way.

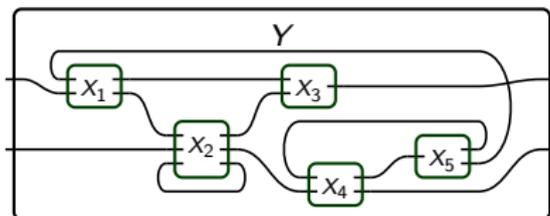
- This requires proof: arbitrary wiring diagrams, arbitrary DS's.^{5 6}

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Steady state plots are compositional

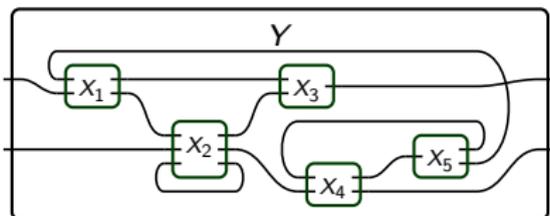
One last compositional mapping: steady state plots.



Start with an ODS in each box

Steady state plots are compositional

One last compositional mapping: steady state plots.



Start with an ODS in each box

- Compute steady states: solution to $\dot{x} = 0$
- Do this for each ODS in the wiring diagram
 - Get a system of equations
 - Plot to get “steady state plots” (a.k.a. bifurcation diagrams)
 - Compose these plots using PA method
- Steady state plots are compositional.
- Steady states of whole = simultaneous steady states of parts

Summary



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 - Operad = “theory of composition”; algebras = models

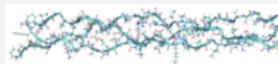
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Questions and comments welcome!