

Applied Category Theory: Mathematics for Interdisciplinary systems modeling

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Outline

1 Introduction

- The fabric of interdisciplinarity
- Our historical moment
- Plan of the talk

2 Operads: a framework for compositional operations

3 Functors connecting operads

4 The Pixel array method

5 Wrapping up

A road to true interdisciplinarity

- Scientific disciplines are conceptual analogies of the world.
 - Science: a schematic, conceptual account of phenomena.
 - Engineering is using these accounts to channel world events.
 - But how do different disciplines and accounts cohere?
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 - Interdisciplinarity consists of effective analogy-making.
 - To go further, we need to formalize the analogies themselves.

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 - Interdisciplinarity consists of effective analogy-making.
 - To go further, we need to formalize the analogies themselves.
- Better yet: we need a conceptual stem-cell.
 - Something that can differentiate into huge variety of forms.
 - Find the analogies between forms as aspects within the stem cell.

Category theory as conceptual stem-cell

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- All forms of pure math... (we'll briefly discuss this)
- Databases and knowledge representation (categories and functors)
- Functional programming languages (cartesian closed categories)
- Universal algebra (finite-product categories)
- Dynamical systems and fractals (operad-algebras, co-algebras)
- Shannon Entropy (operad of simplices)
- Partially-ordered sets and metric spaces (enriched categories)
- Higher order logic (toposes = categories of sheaves)
- Measurements of diversity in populations (magnitude of categories)
- Collaborative design (enriched categories and profunctors)
- Petri nets and chemical reaction networks (monoidal categories)
- Quantum processes and NLP (compact closed categories)

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- Couldn't the same objection be made about mathematics?
 - Mathematics is the basis of hard science, used everywhere.
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 - Conclude that math/CT explains everything and hence nothing?
- Stem cells don't do work until they differentiate.
 - “Adult-level” work requires differentiation and optimization.
 - But the unified origins lead to impressive interoperability.

CT is the mathematics of mathematics.

You could also say: CT is mathematics, self-aware.

- Designed to transport theorems from one area of math to another.
 - From topology (shapes) to algebra (equations).
 - This isn't mere analogy, it's analogy made rigorous.

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 - Most modern pure math research is written cat.-theoretically.
 - It's become a gateway to pure mathematics.
- And it's branched out from math in a big way.
 - Databases and knowledge representation ([categories and functors](#))
 - Functional programming languages ([cartesian closed categories](#))
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If you care about information hygiene, CT needs to be on your radar.

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Let's focus on one.

- Operads: the category-theoretic formalization of “operations”.
- A branch of category theory that well represents the spirit.
- “Operadic”: a *theme* of design patterns.

Plan of the talk

I'll discuss CT as mathematics for organizing information.

- *Operads*, a general framework for compositional operations.
 - I'll sketch a definition and give a lot of examples.
 - Functors between operads connect different operation domains.
 - Application: solving simultaneous systems of nonlinear equations.

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Let's get into it with *operads*, a framework for compositional operations.

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- 2 Operads: a framework for compositional operations**
 - Operads: e pluribus unum
 - Examples of operads
- 3 Functors connecting operads
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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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- Operads structure this sort of thinking.
- With mathematical structure, we can go much further.

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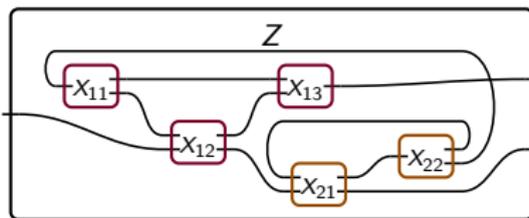
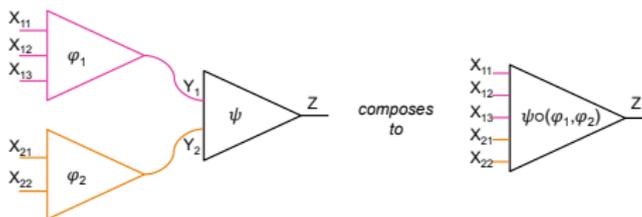
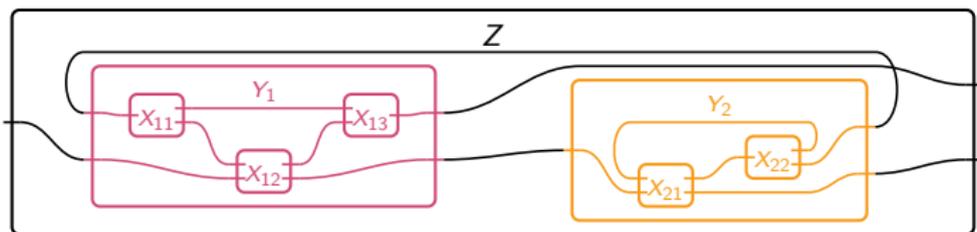
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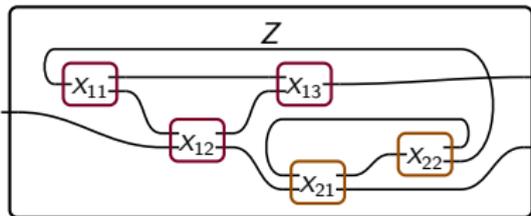
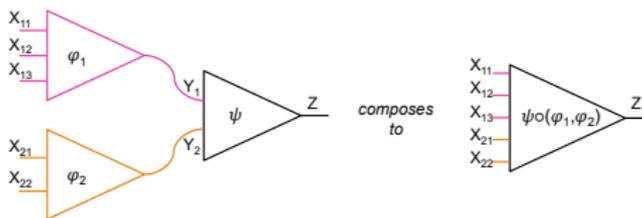
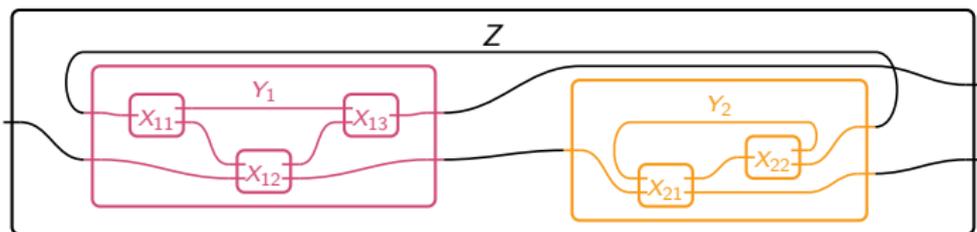
Let's look for **sorts**, **arrangements**, and **nesting** in some examples.

Operad 1: wiring diagrams



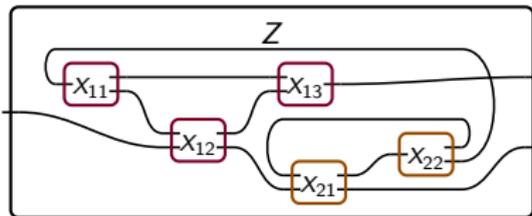
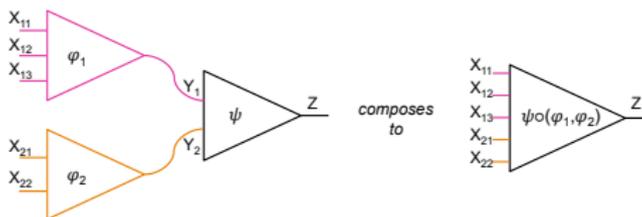
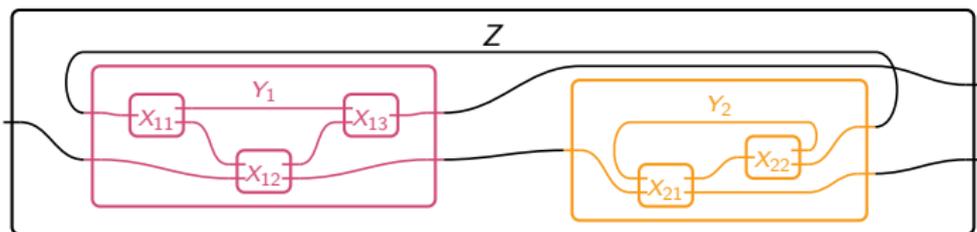
Sorts: boxes with ports.

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Sorts: boxes with ports. **Arrangements:** wiring diagrams.

Operad 1: wiring diagrams



Sorts: 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 *sorts*.
- For sorts $X_1, \dots, X_k, Y \in \text{Ob}(\mathcal{O})$, 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 .
A k -ary 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 sort $X \in \text{Ob}(\mathcal{O})$, 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:

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



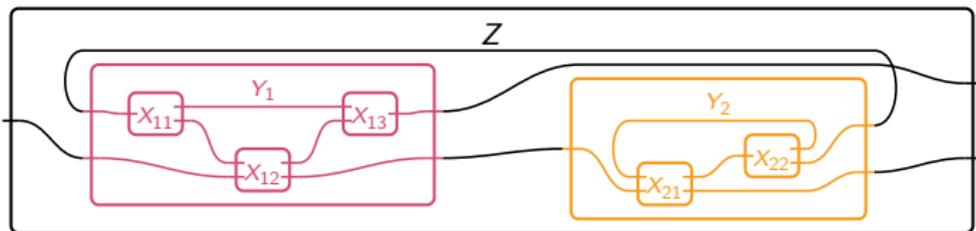
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- Arrangement $\varphi: X_1, \dots, X_k \rightarrow Y$ in \mathcal{W} : any **wiring** of X 's in Y .
- Nesting: the facts about this **fractal** of wiring possibilities.



\mathcal{W} provides fine-grained control of flow operators and operations.

Operad 2: hierarchical protein materials

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

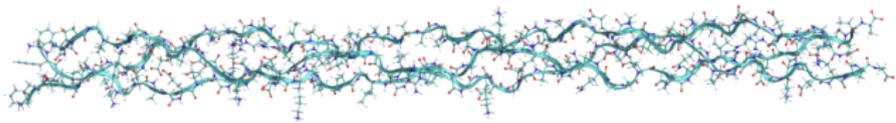
- A **protein** is an **arrangement** of simpler **proteins**.
 - There are “atomic” proteins: amino acids.
 - Protein materials include your skin: stretchable, breathable, waterproof.
 - Materials scientists would *love* to make materials like this.

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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- 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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Operad 3: probabilities

Even an operad with **one sort** can be interesting.

- Call the operad \mathcal{P} for “probabilities”
- Give it one **sort** E for “event”.
- All that matters are **arrangements** $\varphi: (E, \dots, E) \rightarrow E$ and **nesting**.

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A k -ary **arrangement** is any distribution of k events in an event.

- That is, $\mathcal{P}_k := \{(x_1, \dots, x_k) \in \mathbb{R}_{\geq 0}^k \mid x_1 + \dots + x_k = 1\}$.

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- Examples:
 - flip coin: $f = (\frac{1}{2}, \frac{1}{2}) \in \mathcal{P}_2$.
 - roll die: $r = (\frac{1}{6}, \dots, \frac{1}{6}) \in \mathcal{P}_6$.
 - pick card: $p = (\frac{1}{52}, \dots, \frac{1}{52}) \in \mathcal{P}_{52}$.

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- The first is an arrangement of head and tail events in coin flip event.
- The **nesting** rule is multiplication:
 - Flip a coin: result decides whether to roll a die or pick a card.

$$f \circ (r, p) = \left(\underbrace{\frac{1}{12}, \dots, \frac{1}{12}}_{6 \text{ times}}, \underbrace{\frac{1}{104}, \dots, \frac{1}{104}}_{52 \text{ times}} \right) \in \mathcal{P}_{58}$$

A zoo of operads: Grammars

Any context-free grammar is an operad.

$\langle \text{sentence} \rangle$	$::=$	$\langle \text{noun-phrase} \rangle \langle \text{verb-phrase} \rangle$
$\langle \text{noun-phrase} \rangle$	$::=$	$\langle \text{pronoun} \rangle \mid \langle \text{proper-noun} \rangle \mid \langle \text{determiner} \rangle \langle \text{nominal} \rangle$
$\langle \text{nominal} \rangle$	$::=$	$\langle \text{noun} \rangle \mid \langle \text{nominal} \rangle \langle \text{noun} \rangle$
$\langle \text{verb-phrase} \rangle$	$::=$	$\langle \text{verb} \rangle \mid \langle \text{verb} \rangle \langle \text{noun-phrase} \rangle \mid \langle \text{verb} \rangle \langle \text{prep-phrase} \rangle$
$\langle \text{prep-phrase} \rangle$	$::=$	$\langle \text{preposition} \rangle \langle \text{noun-phrase} \rangle$

How is this an operad?

- The **sorts** are the parts of speech.
- The **arrangements** are the production rules.
- **Nesting** is nesting.

The operad of sets

There is an operad **Set** of sets and functions.

- The **sorts** in **Set** are all the sets, e.g. $\{r, g, b\}$, \mathbb{N} , \mathbb{R}^2 , etc.
- An **arrangement** is a function $f: X_1 \times \cdots \times X_k \rightarrow Y$.
- **Nesting** is composition $f \circ (g_1, \dots, g_k)$.

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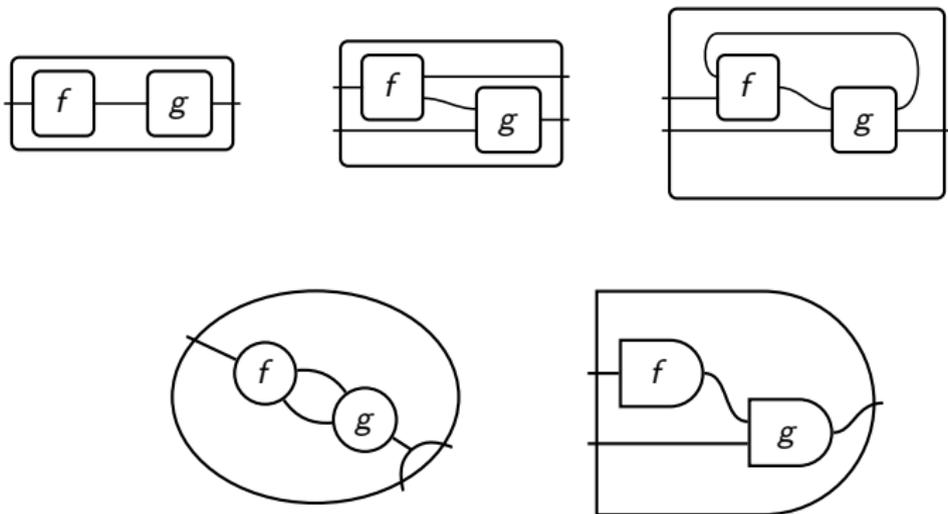
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Think of sets as containing features one can sort into.

- An **arrangement** sorts a k -dimensional feature space into one dimension.

Wiring diagram operads, similar to #1

A representative **arrangement** $\varphi: X, Y \rightarrow Z$ in five WD operads.



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 - Algebras: what we are composing
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Functors translate between operads

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- protein materials,
- sets,
- probabilities,
- grammars.

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A functor $F: \mathcal{O} \rightarrow \mathcal{O}'$ is a translator from one operad to another.

- Functors between grammars are like compilers, or elaborations.
- Functors between wiring diagram operads are sub-languages.
- Functors $\mathcal{O} \rightarrow \mathbf{Set}$ are special: they're called *\mathcal{O} -algebras*.

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Algebras *operationalize* operads.

Operads and their algebras

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- Operad : Group theory :: Algebras : Groups.
- Operad : Ring theory :: Algebras : Rings.

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Operad = theory. Algebras = models.

Each operad has many algebras

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

- **Sorts** 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 $A: \mathcal{O} \rightarrow \mathbf{Set}$ are the models of theory \mathcal{O} .

- An \mathcal{O} -algebra A says what's actually being composed.
 - To each **sort** X : a set $A(X)$ of elements.
 - To each **arrangement** φ : a k -ary operation $A(\varphi)$.
 - If $\varphi: X_1, \dots, X_k \rightarrow Y$ is an arrangement,
 - Then $A(\varphi): A(X_1) \times \dots \times A(X_k) \rightarrow A(Y)$ is a function.
 - To each **nesting**: a law in A .

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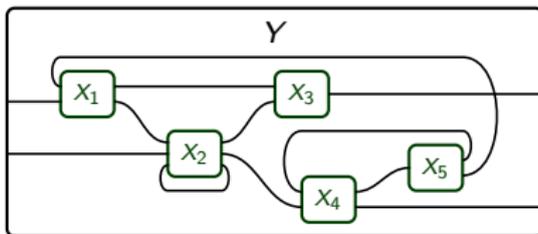
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Next, I'll explain what algebras on an operad look like.

Multiple algebras for wiring diagrams operad

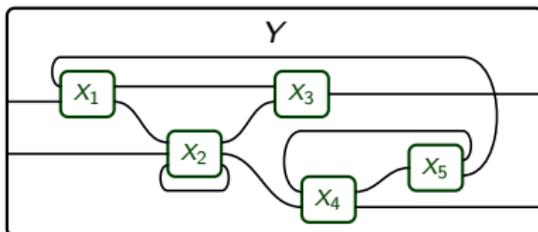
Recall operad \mathcal{W} of all boxes X and WDs, $\varphi: X_1, \dots, X_5 \rightarrow Y$.²



²Imagine each port / wire labeled by a topological space: the signal space.

Multiple algebras for wiring diagrams operad

Recall operad \mathcal{W} of all boxes X and WDs, $\varphi: X_1, \dots, X_5 \rightarrow Y$.²

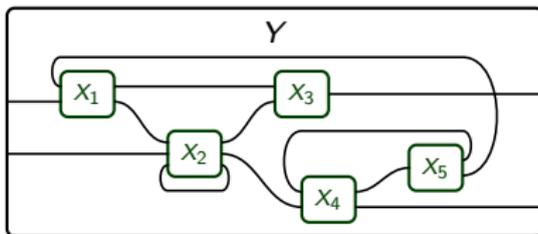


There are many different \mathcal{W} -algebras $A: \mathcal{W} \rightarrow \mathbf{Set}$.

²Imagine each port / wire labeled by a topological space: the signal space.

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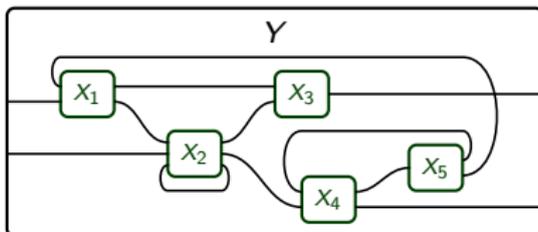
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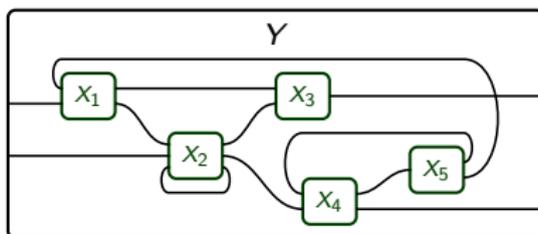
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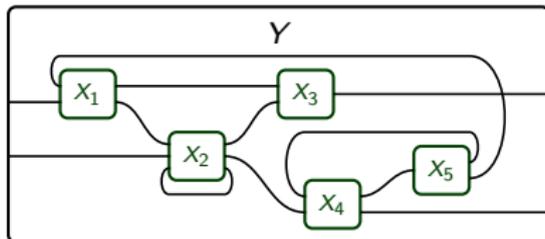
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- But there's a much simpler "algebraic" algebra...

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\mathcal{W} -algebra of tensor networks

We said \mathcal{W} is modeled by dynamical systems.



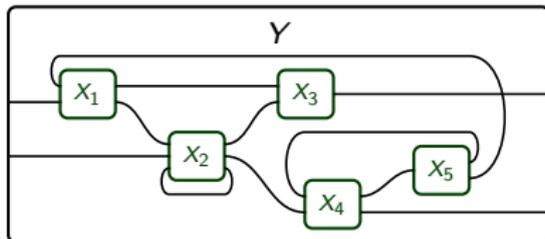
Another algebra $\mathcal{W} \rightarrow \mathbf{Set}$: tensors (not dynamic at all).³

- Box = tensor format ($T \in V_1 \otimes \cdots \otimes V_n$).
- Wiring diagram = tensor network.
- Contract along shared wires to “compose”.

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Later: a relationship between dynamical systems and tensors...

- ... which led me to a numerical method for solving systems.
- The pixel array method, up next.

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Outline

- 1 Introduction
- 2 Operads: a framework for compositional operations
- 3 Functors connecting operads
- 4 The Pixel array method**
 - The basic picture
 - Wiring diagrams
 - Speed, accuracy, and applications
- 5 Wrapping up

Detailed look at a real-world application

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

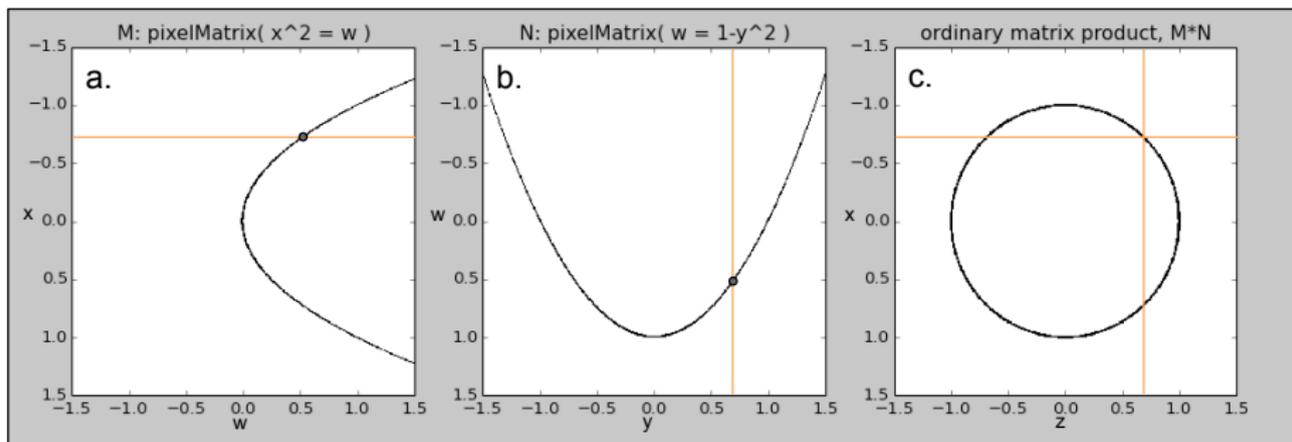
- Plot each in a bounding box, e.g. $[-1.5, 1.5]$.
- Consider plots as matrices of on/off pixels (booleans).
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Example: $x^2 = w$ and $w = 1 - y^2$.



A more complex example

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

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

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

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

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

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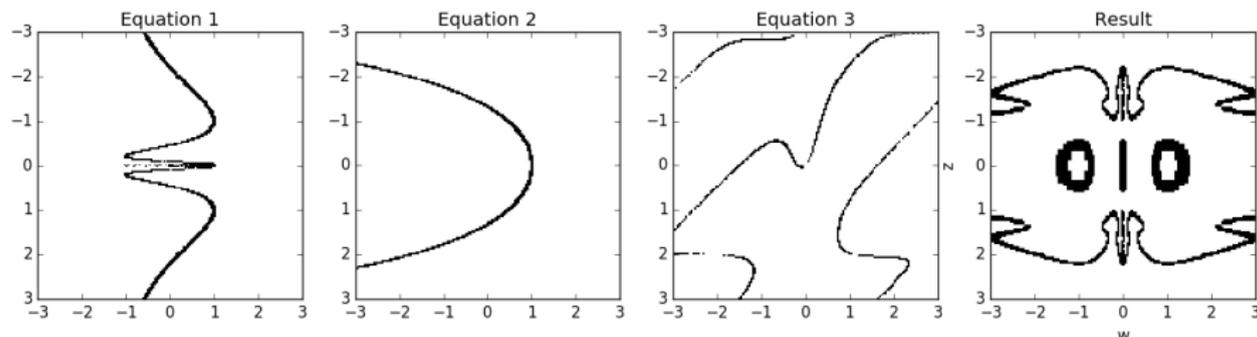
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Equations and wiring diagrams

Consider an arbitrary system of equations having the following form:

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

$$f_2(\mathbf{v}, w, x) = 0$$

$$f_3(u, w, x, y) = 0$$

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

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

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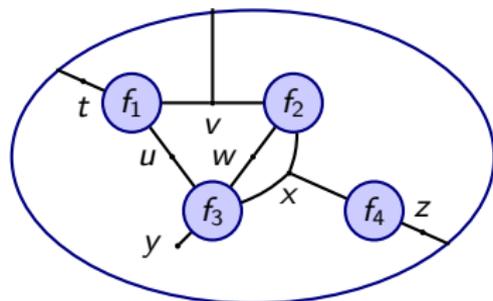
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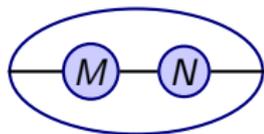


Said another way, we want $\{(t, v, z) \mid \exists u, w, x, y : f_1 = f_2 = f_3 = f_4 = 0\}$.

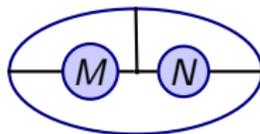
Example wiring diagrams for named operations

Some famous matrix products as wiring diagrams:

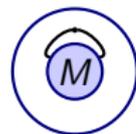
Multiplication: MN



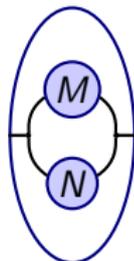
Khatri-Rao: $M \odot N$



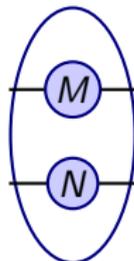
Trace: $\text{Tr}(M)$



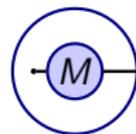
Hadamard: $M \circ N$



Kronecker: $M \otimes N$



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



Speed and accuracy

- The PA method has good accuracy guarantees.
 - No false negatives, only false positives.
 - As pixel density $\rightarrow \infty$, false positive $\rightarrow 0$
 - Rate is proportional to size of largest derivative.
- The PA method is faster than Newton-style methods....
 - If you want all solutions in a bounding box...
- Applications: plot steady states of dynamical systems.

PA method for dynamical systems

“We can use the PA method to find the steady states of dynamic systems.”

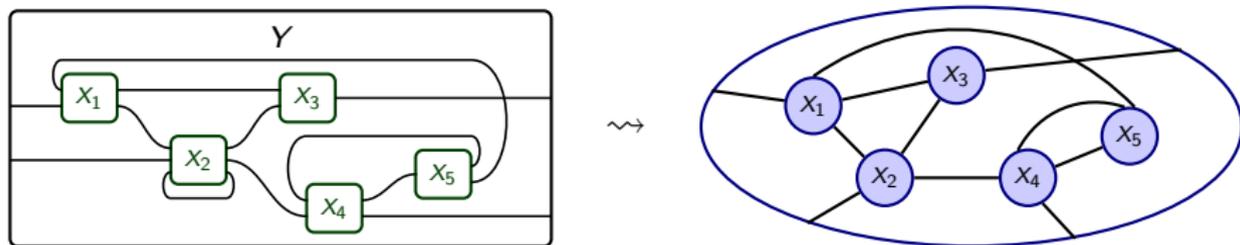
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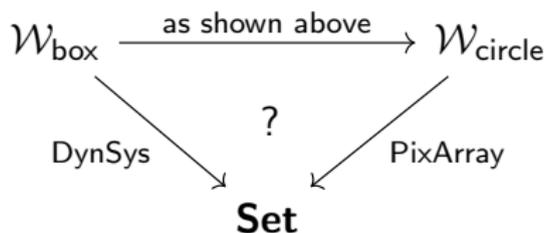
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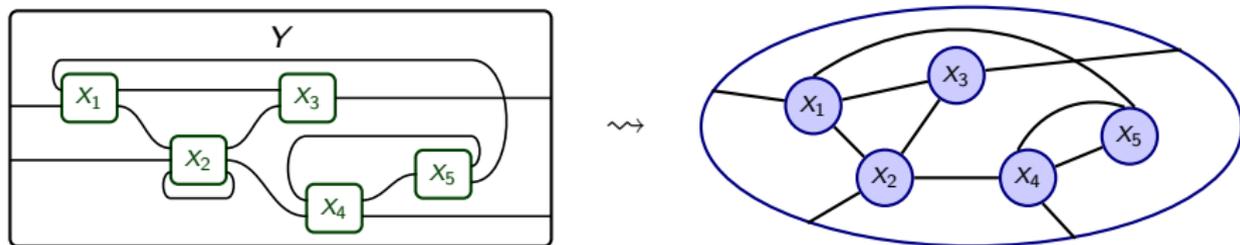


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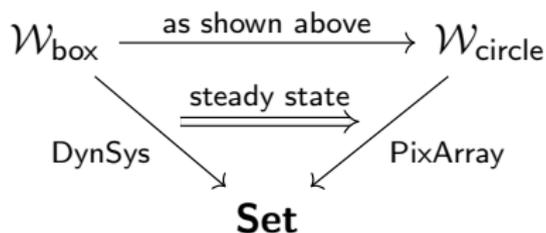
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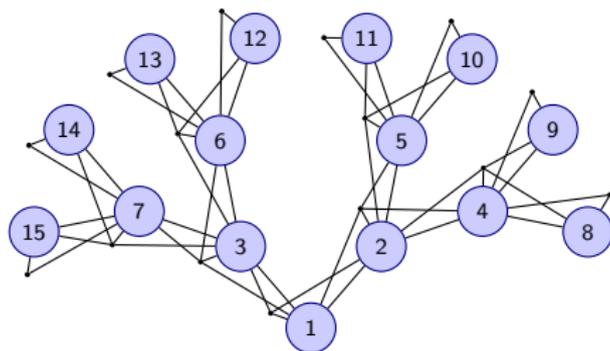
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- This is perfect for the PA method.



- Given parallel resources, runtime is logarithmic in # nodes.

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 - What just happened?
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- We briefly discussed maps between functors.
 - Steady states of dynamical systems arranged as tensors.
 - (Another example: discretization of cont's dynamical systems.)

Ok, but why did that happen?

The point of all that was to give a glimpse into category theory.

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There's even a category of categories and an operad of operads.

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A science of interdisciplinarity can reduce waste.

- Models of different systems need to be **independent** to optimize.
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