Category theory in science and engineering: A framework for information integration

David I. Spivak

Mathematics Department
Massachusetts Institute of Technology

November 15, 2017

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  - It arises from multiple sources and perspectives;
  - It must be integrated to solve larger problems.

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  - Making connections, drawing analogies.
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- Composition, similar to integration:
  - Putting components together.
  - Interconnecting complex systems.
  - Finding common structures across scales.

How category theory fits in

Integration and composition:

- Driving in the car.
- Listening to a talk.
- Or in synthetic biology, e.g. molecular biology + electrical engineering.

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...CT is a discipline that focuses on *integration* as its *subject*.

- Translates between disciplines.
- Classifies relationships between objects.
- Manages what is preserved vs. lost in translation.
- Focuses on composition: putting things together.

Why apply category theory?

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- internet of things,
- cyber-physical systems,
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Category theory can help organize this complexity.

- CT's organizational power is well-known in pure math.
- People—myself included—have been pushing it into other fields.
- Engineering, CS, materials sci., manufacturing, oceanography, cog-sci.

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- Engineering, CS, materials sci., manufacturing, oceanography, cog-sci.
- NASA example: need accurate, timely decision amid great complexity.

Plan of the talk

I'll discuss CT as mathematics for organizing information.

- 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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  - I'll give examples and sketch a definition.
  - Operads: the mathematical framework for the talk.
- Application of CT to studying systems:
  - Systems of equations: a new numerical method.
  - Information systems: combine data from disparate sources.
  - Dynamical systems: compositional analyses.

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- And ways to arrange them, $\varphi\colon X_1, \ldots, X_k \to Y$,
- Such that arrangements can be nested inside each other.

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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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- There’s a common theme in the way we think.
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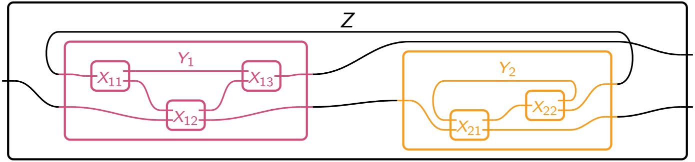
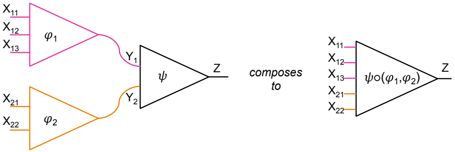
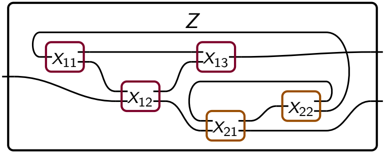
Let's look for objects, arrangements, and nesting in some examples.

Operad 1: wiring diagrams







Objects: boxes with ports.

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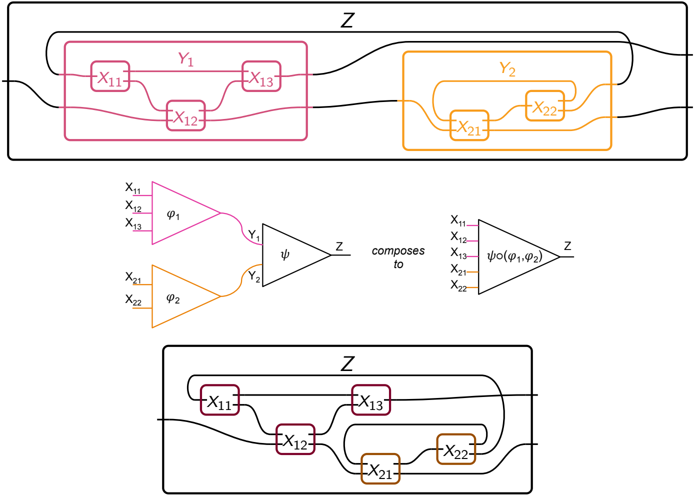

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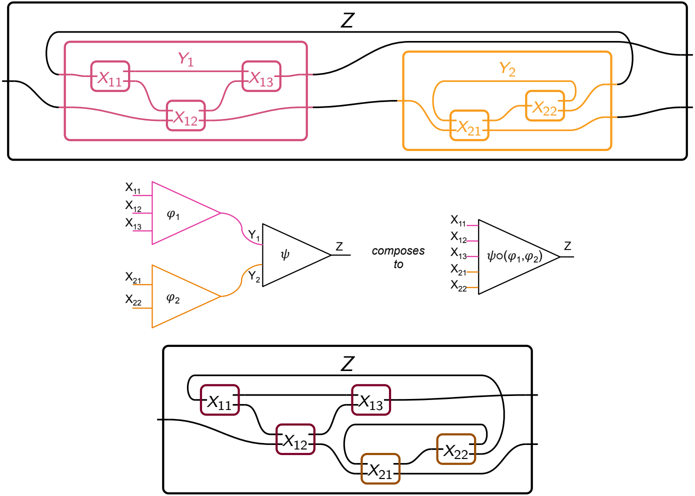


Objects: boxes with ports. Arrangements: wiring diagrams. Nesting: nesting.

Formal definition of operad

An operad $\mathcal{O}$ consists of

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

  $$\mathrm{Mor}_{\mathcal{O}}(X_1, \ldots, X_k; Y)$$

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

  $$\varphi\colon X_1, \ldots, X_k \to Y.$$

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

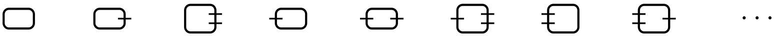
  $$\psi \circ (\varphi_1, \ldots, \varphi_k)\colon (X_{i,j}) \xrightarrow{\varphi_i} (Y_i) \xrightarrow{\psi} Z.$$

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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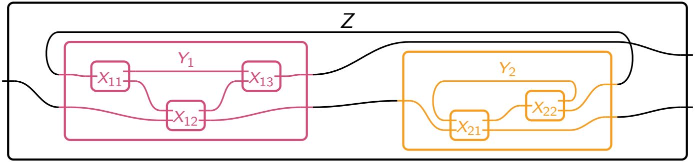
$\cdots$

- Arrangement $\phi\colon X_1, \ldots, X_k \to Y$ 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.

[1] Giesa, 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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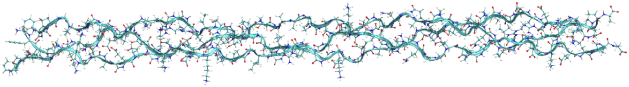
- Assemble new proteins from old:
  - arrange in series or parallel (H-bonds), or
  - arrange in helices, double helices, any conceivable curve, etc.



- 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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More operads: Grammars and recipes

Context-free grammars are “free” operads.

$$
\begin{aligned}
\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 \\
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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.

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 $X, Y, \ldots$: what *sorts* of elements in this theory?
- Arrangements ϕ, ψ: what are the operations?
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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 $\phi \colon X_1, \ldots, X_k \to Y$ is an arrangement,
    - Then $A(\phi) \colon A(X_1) \times \cdots \times A(X_k) \to A(Y)$ is a function.
  - To each nesting: a law in A.

[2]Technically, an algebra is a functor $A \colon \mathcal{O} \to \mathbf{Set}$.

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

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Example: the operad for monoids

Monoids are groups without inverses.

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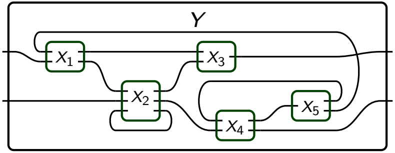
- The operad laws (unitality, associativity) guarantee the monoid laws.

The simplest operad is the one for monoids.

Multiple algebras for wiring diagrams operad

Recall operad $\mathcal{W}$ of all boxes X and WDs, $\phi\colon X_1, \dots, X_k \to Y$.[3]



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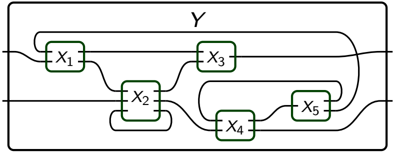

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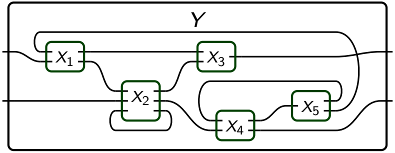

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  - $A(X)$: the set of all DS's with input-output shape X.
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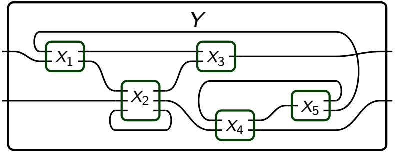

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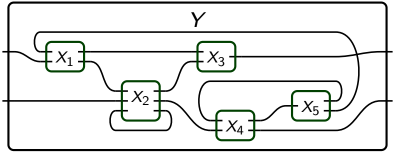

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- But there's a much simpler "algebraic" algebra...

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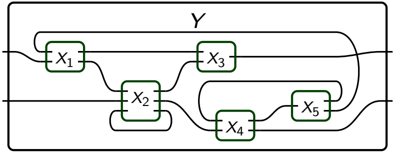
Tensors are a $\mathcal{W}$-algebra

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



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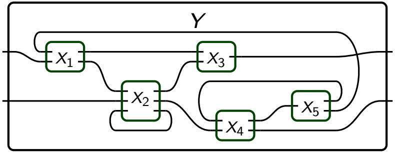

But $\mathcal{W}$ is also modeled by tensors (not dynamic at all).[4]

- 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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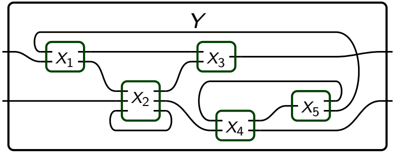

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Next up: using this algebra for solving general systems of equations.

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Detailed look at an 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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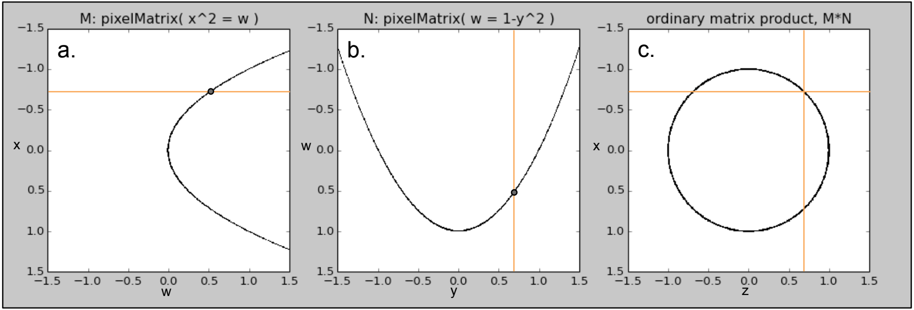
Example: $x^2 = w$ and $w = 1 - y^2$.



A more complex example

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

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

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

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

Q: For what values of w and z does a simultaneous solution exist? [5]

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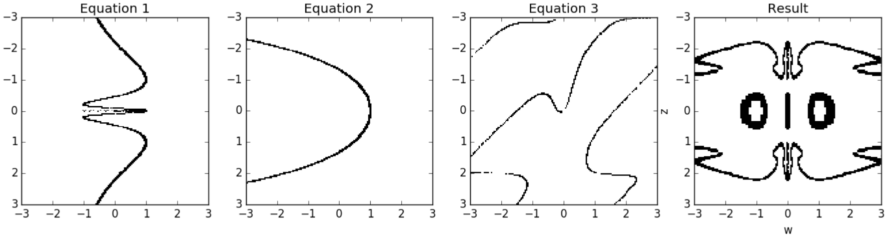

[5] Spivak; Dobson; Kumari; Wu (2016) "Pixel Arrays: A fast and elementary method for solving nonlinear systems". https://arxiv.org/abs/1609.00061

Equations and wiring diagrams

Consider an arbitrary system of equations having the following form:

$$\begin{aligned} f_1(\mathbf{t}, u, \mathbf{v}) &= 0 \\ f_2(\mathbf{v}, w, x) &= 0 \\ f_3(u, w, x, y) &= 0 \\ f_4(x, \mathbf{z}) &= 0 \end{aligned}$$

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

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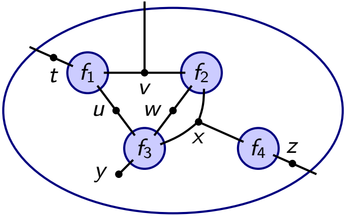
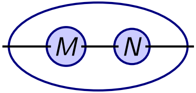


Said another way, we want $\{(t, v, z) \mid \exists u, w, x, y : f_1 = f_2 = f_3 = f_4 = 0\}$.

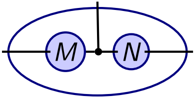
Example wiring diagrams for named operations

Some famous matrix products as wiring diagrams:

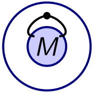
Multiplication: MN



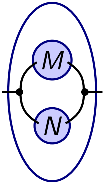
Khatri-Rao: $M \odot N$



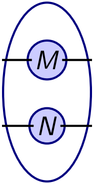
Trace: $\mathrm{Tr}(M)$



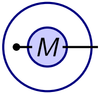
Hadamard: $M \circ N$



Kronecker: $M \otimes N$

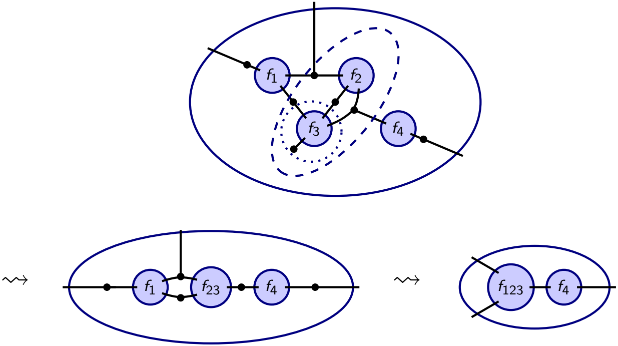


Marginalize: $\sum_i M_{i,j}$



Clustering for speed

To solve systems of equations fast, cluster:



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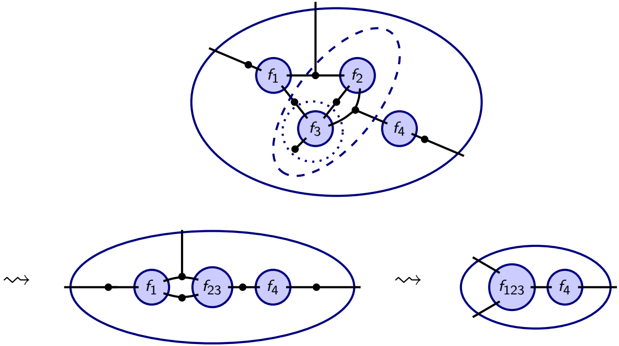

The operad associative law lets you choose the order.

- 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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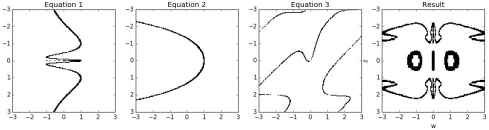

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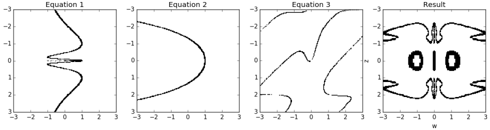

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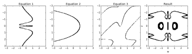
Above case: PA was over 7200x faster.

- 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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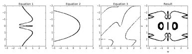

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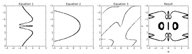

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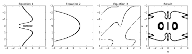

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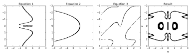
- PA method: multiply plots as tensors.
- Result (solution) has the same guarantees:
  - If there is a solution in a pixel, it is marked.
  - If a pixel is marked, then the pixel is 2ϵ-close to a solution.

Other selling points of the PA method



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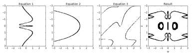

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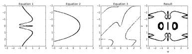

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    - Example: $([0, \infty], \min, \max)$, "save the ϵ's."
    - Monotonic: zoom in and out.
    - Multilinear: amenable to tensor decompositions.

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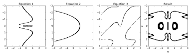

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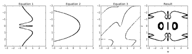

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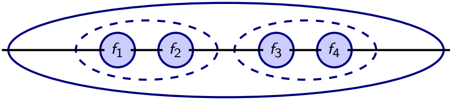
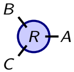
- Compositional: solve one piece now, use it later.



The PA idea is not particular to equations

Data often comes in the form of relations $R \subseteq A \times B \times C$.



A	B	C
1	r	3.77
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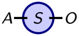
1	s	2.04
2	r	4.90
2	s	2.18
⋮	⋮	⋮
4	s	6.18



Attrib. / **Obj.**	a_1	a_2	a_3	a_4
o_1		•	•	
o_2	•	•	•	
o_3			•	•
o_4				
o_5	•		•	
o_6			•	•
o_7		•	•	•

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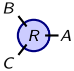

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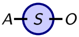

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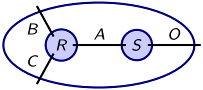
Relations form an $\mathcal{W}$-algebra.



"Find all (b, c, o) for which a match exists in A"

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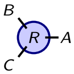

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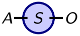

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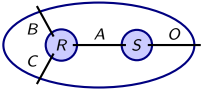
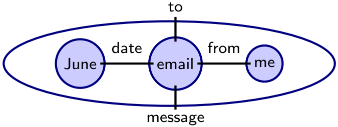


"Find all (b, c, o) for which a match exists in A"

I've co-founded a CT-based data integration company.

The value of a mathematical language

The operad structure is everywhere:



- Bridge formal math and casual users.
- The same formalism, many uses.
  - Data (relations) form a $\mathcal{W}$-algebra.
  - Matrices form a $\mathcal{W}$-algebra.
  - Dynamical systems form a $\mathcal{W}$-algebra.
  - Compositional neural networks form a $\mathcal{W}'$-algebra.

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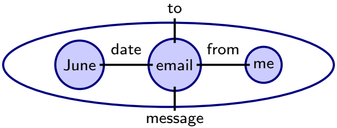

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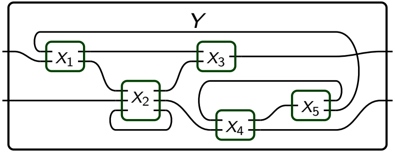
  - Compositional neural networks form a $\mathcal{W}'$-algebra.
- Category theory considers relationships between these algebras.
  - "Compositional mappings".
  - This is our final topic.

Compositional mappings

Suppose there's a continuous DS in each box:



Two choices; what's the difference?

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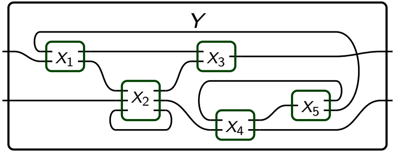

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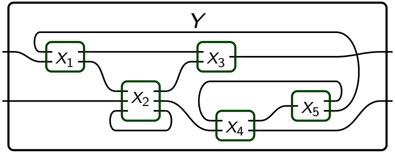
"Discretization is compositional": you get the same result either way.

- This requires proof: arbitrary wiring diagrams, arbitrary DS's.
- I proved it for Euler;[6] my student proved it for Runge Kutta.[7]

[6] Spivak "The steady states of dynamical systems". *arXiv* 1512.00802.
[7] Ngotiaoco "Compositionality of the Runge-Kutta Method". *arXiv* 1707.02804.

Bifurcation diagrams are compositional

One last compositional mapping: bifurcation diagrams.



Bifurcation diagram: plot of steady states.

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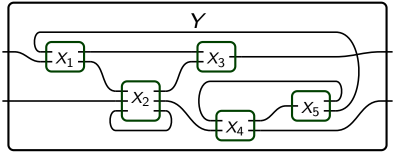
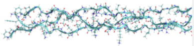
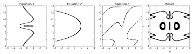


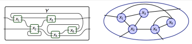
Bifurcation diagram: plot of steady states.

- Steady states: solution to $\dot{x} = 0$.
- Do this for each DS in a wiring diagram.
  - Get a system of equations.
  - Their plots are bifurcation diagrams.
  - Compose these plots using PA method.
- Bifurcation diagrams are compositional.
- Steady states of whole = simultaneous steady states of parts.

Summary



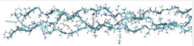


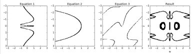


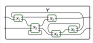
Category theory, and operads, as a framework for information integration.

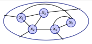
- Operads give a framework for composing things of any sort.
  - Object (interface), morphism (arrangement), composition (nesting).
  - Discussed wiring diagrams, protein materials, grammars, recipes.
  - Operad = "theory of composition"; algebras = models.

Summary









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Go further by adding mathematical structure to complex systems.

- Solving systems of equations: pixel array method.
- Information integration: combine data from disparate sources.
- Interconnect dynamic systems: NASA example.
- Bifurcation theory is compositional for dynamical systems.