Differentiation of stateful functions

Shin-ya Katsumata and David Sprunger*

ERATO MMSD Colloquium
February 7, 2019

Outline

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Ordinary functions as diagrams

We depict functions as boxes with input/output wires. For example, multiplication $\times : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ and copying $\Delta_{\mathbb{R}} : \mathbb{R} \to \mathbb{R} \times \mathbb{R}$ are:

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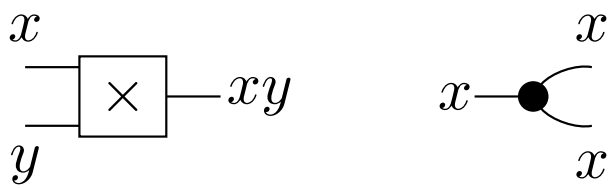

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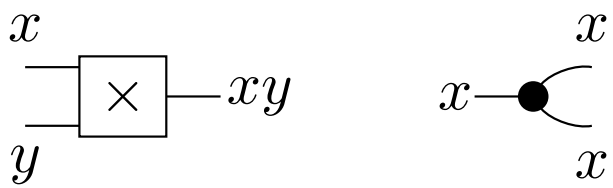

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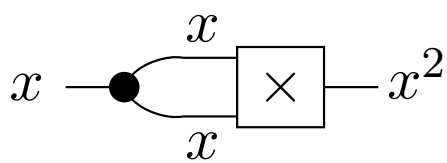

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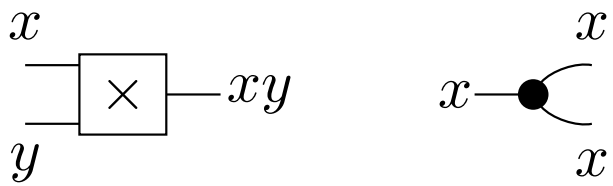

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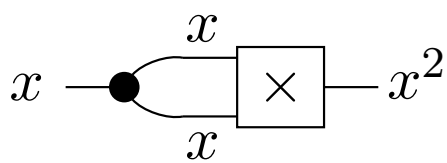
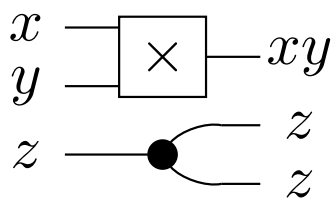
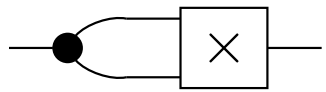


We can also compose functions in parallel:



Functions on sequences, part I

Ordinary functions can be upgraded to functions on sequences:

Input	**Output**
1	
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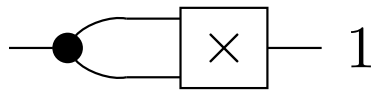
1	 1
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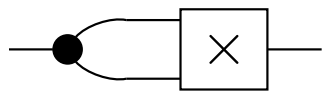
2	
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Input	**Output**
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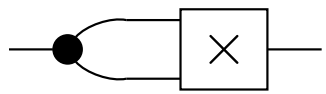

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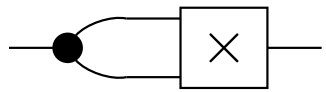
3	
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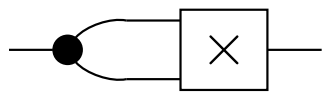

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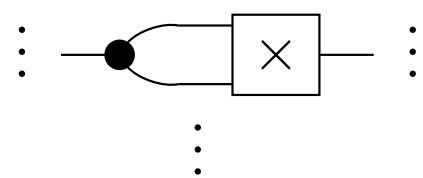

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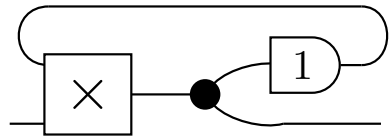
1	
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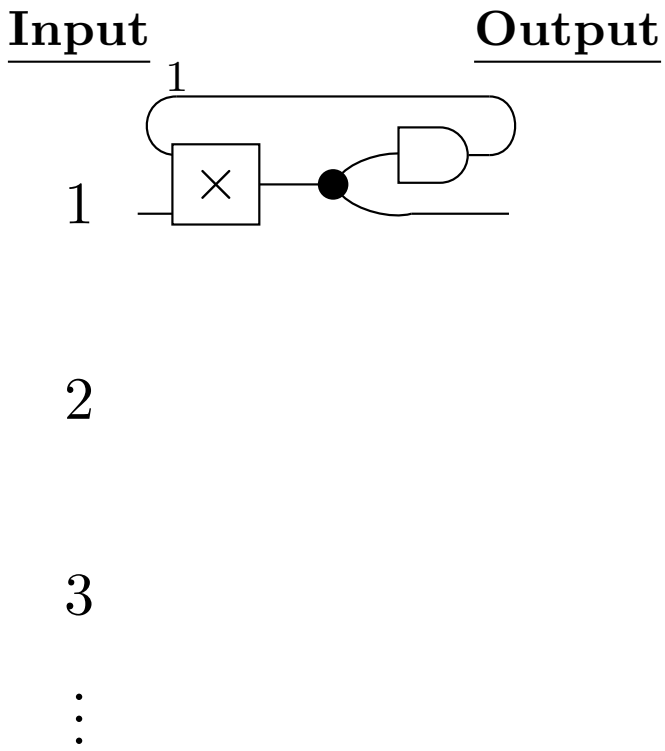

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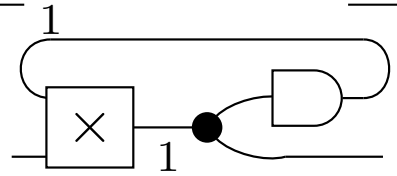
1	
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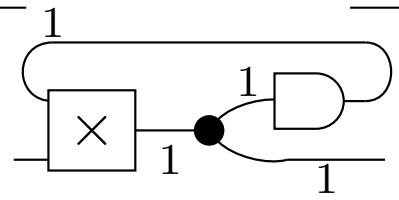
1	
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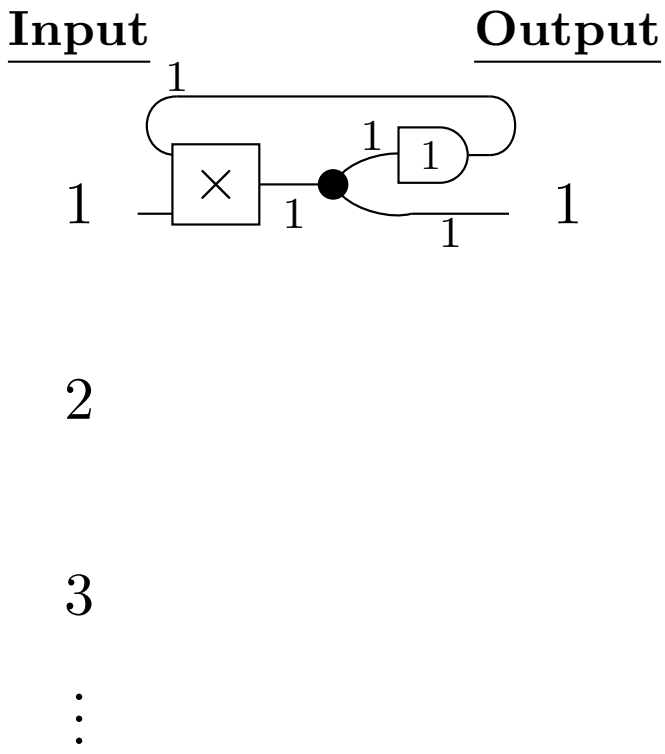

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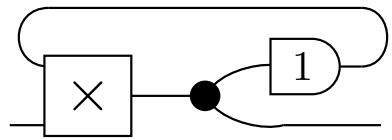
2	
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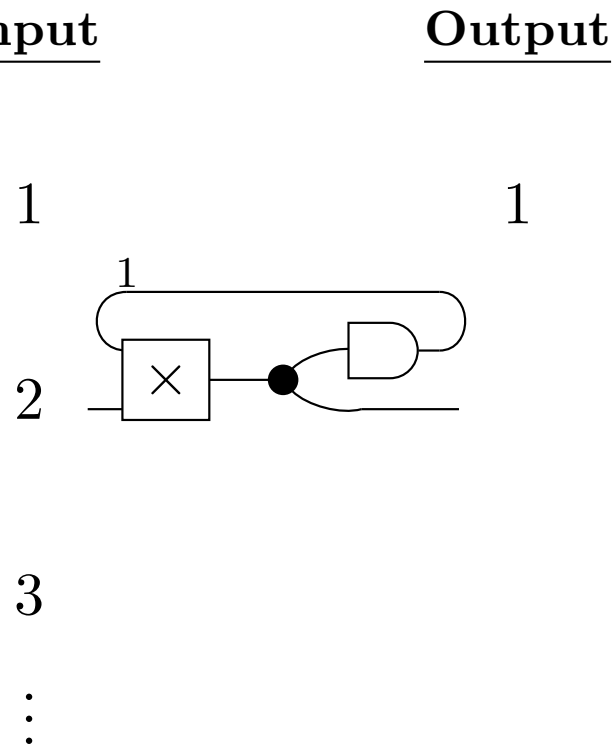

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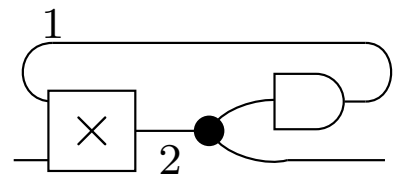

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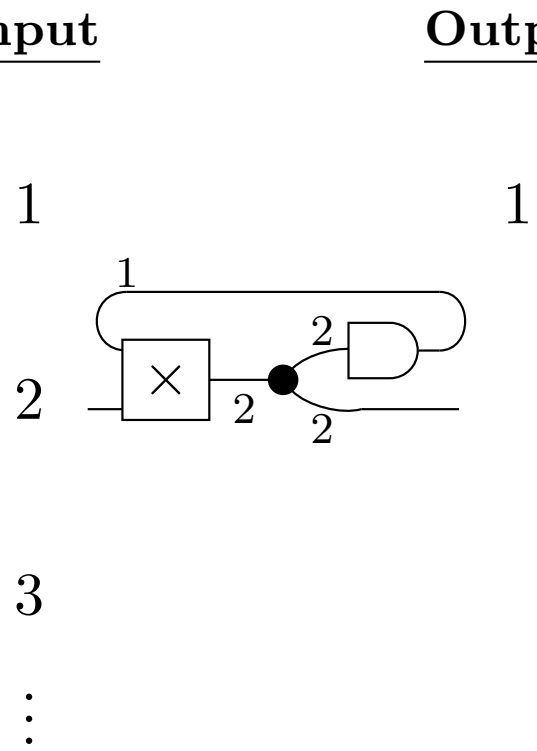

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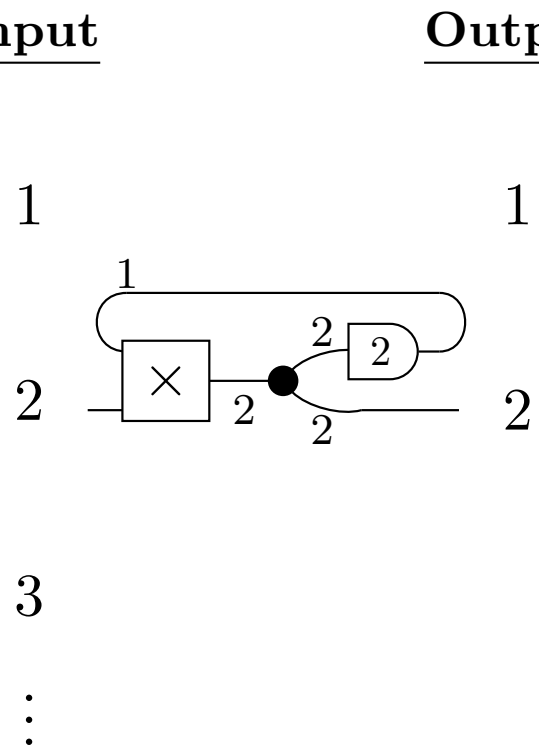

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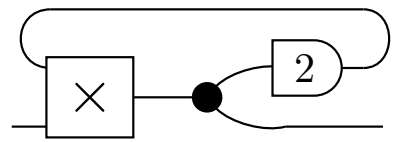
3	
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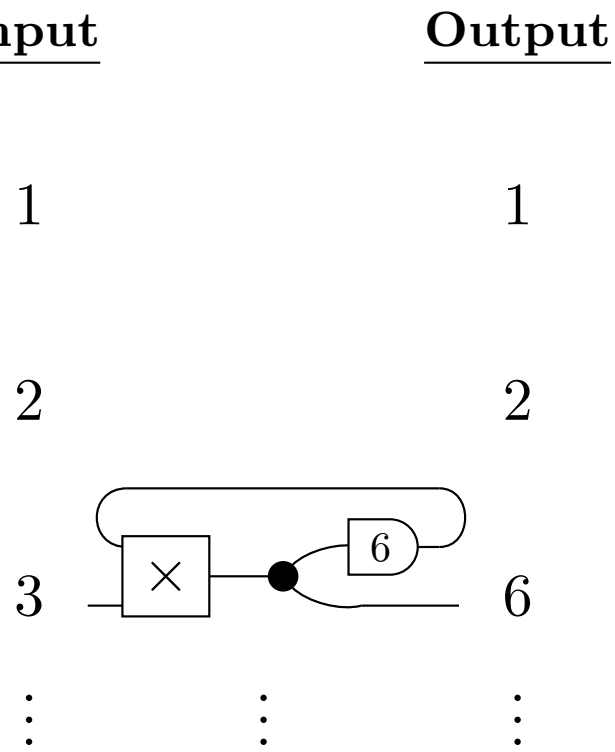

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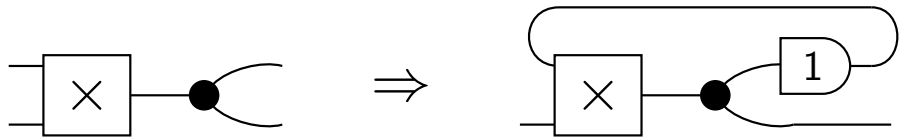
What do diagrams like this, or operational semantics shown previously, remind you of?



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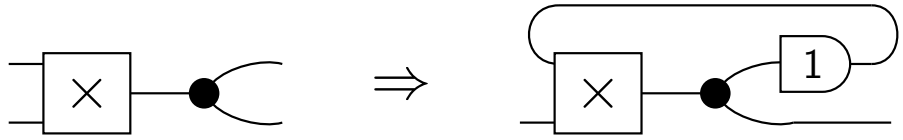
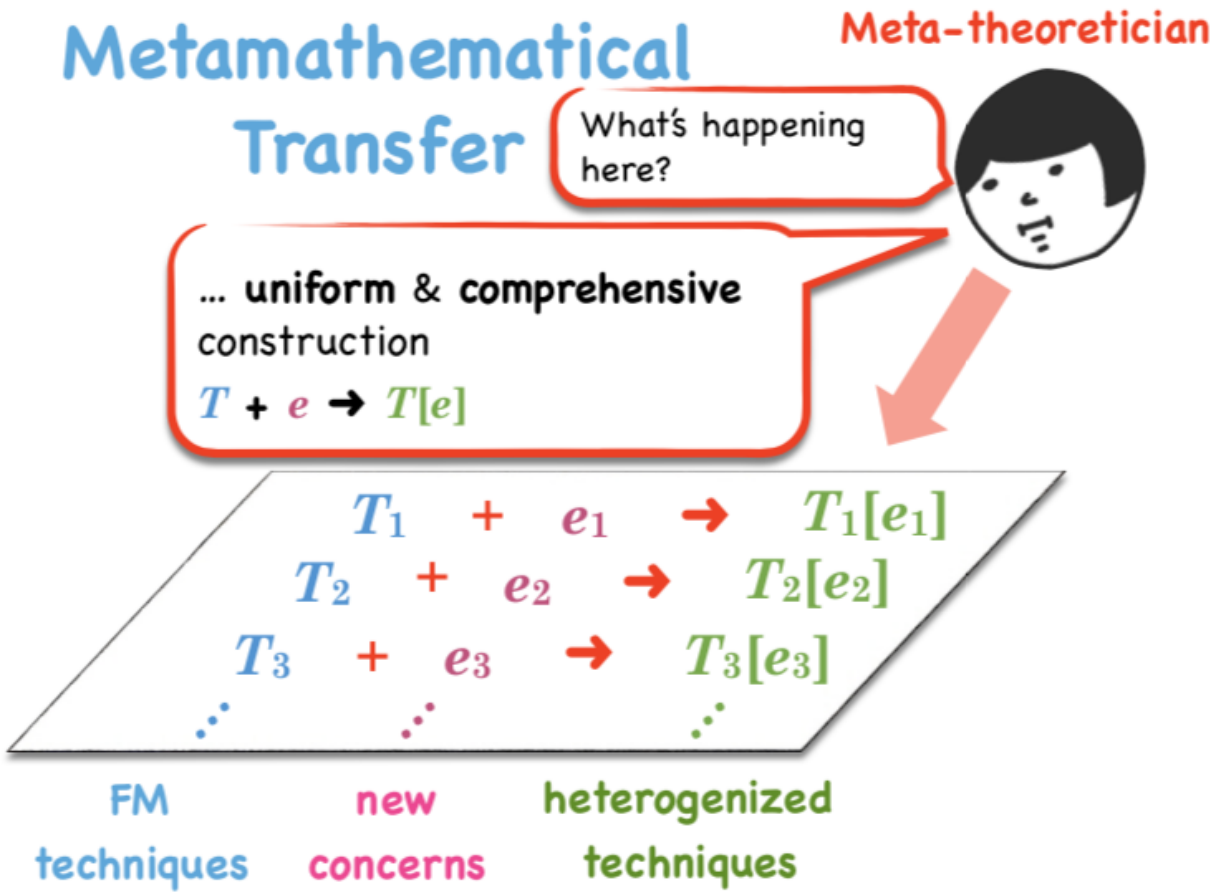


ahem



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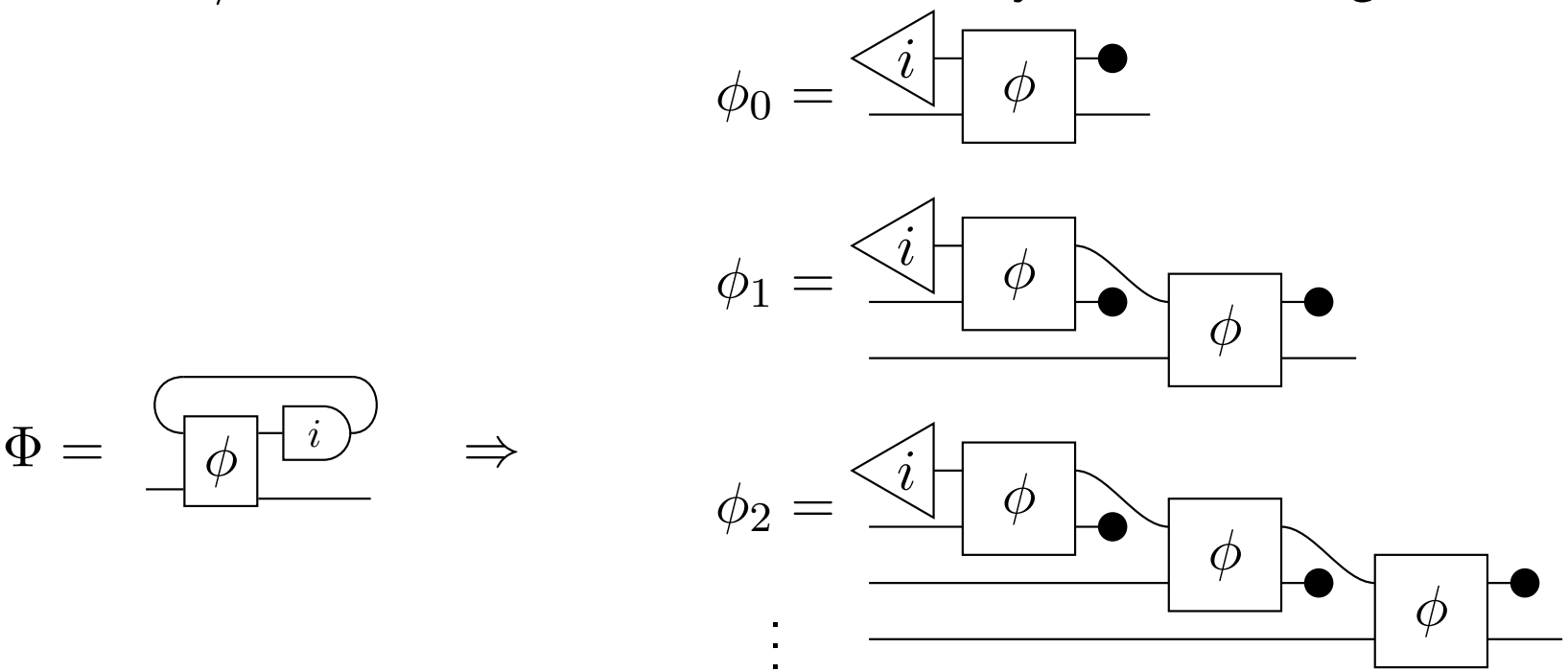

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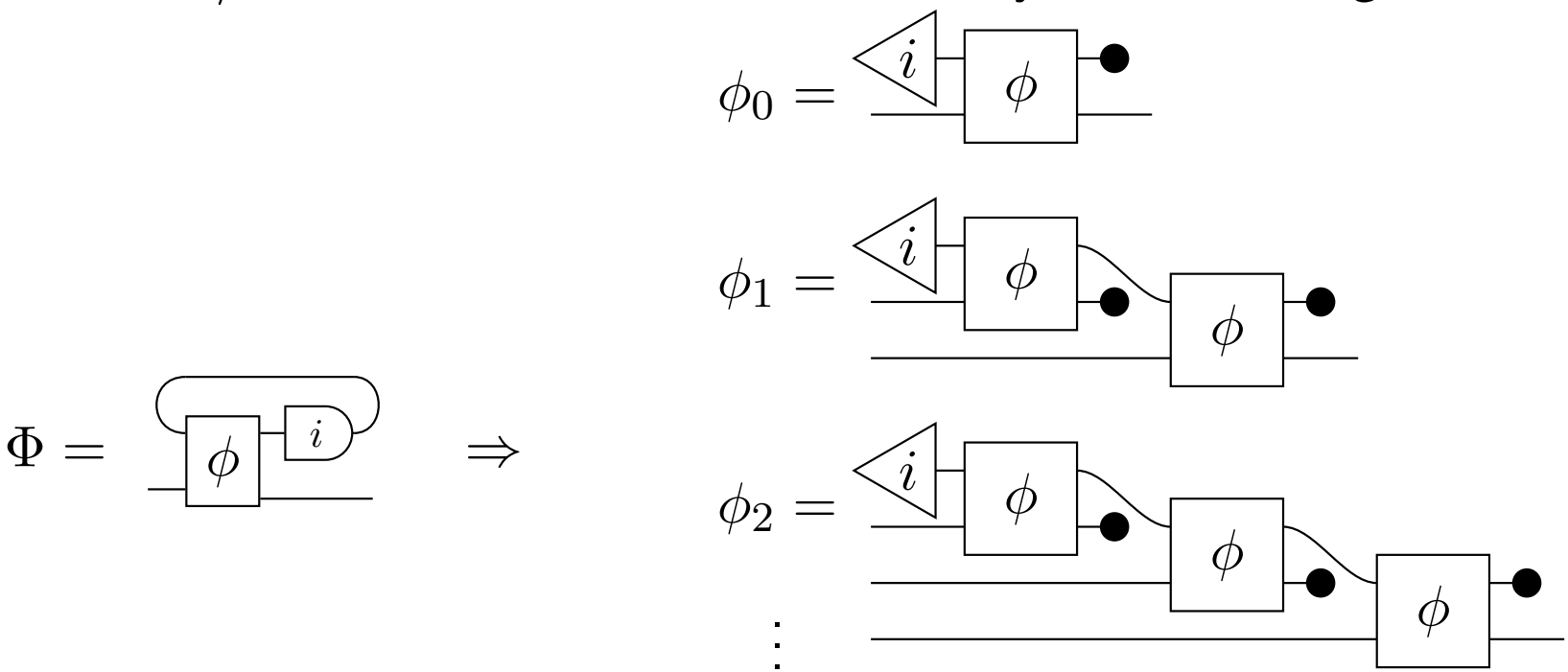

Backpropagation through time (BPTT): Whenever the derivative of Φ is needed at an input of length $k+1$, the derivative of ϕ_k is supplied instead.

Does BPTT make sense, or is it just a hack?

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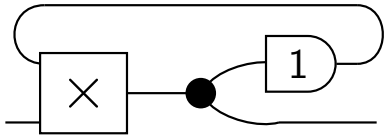
"Making sense" means having the usual properties of derivatives:

1. a sum rule,
2. a chain rule,
3. being linear when evaluated at any base point,
4. symmetry of mixed partial derivatives,

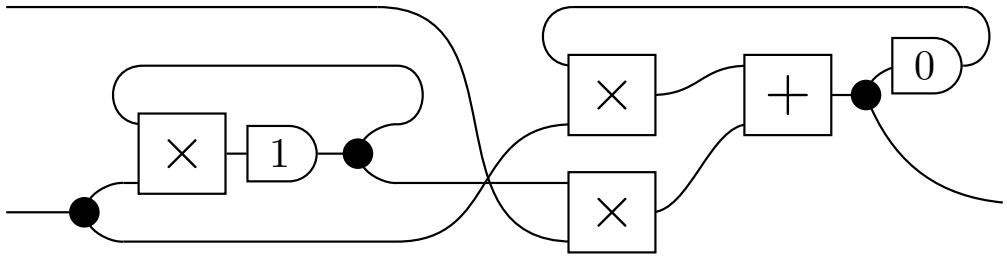
⋮

Outline

Goals of this talk (specific to general)

A. The derivative of 

is this monster



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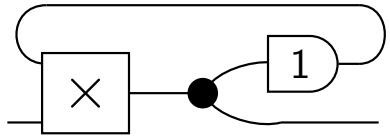
A. The derivative of 

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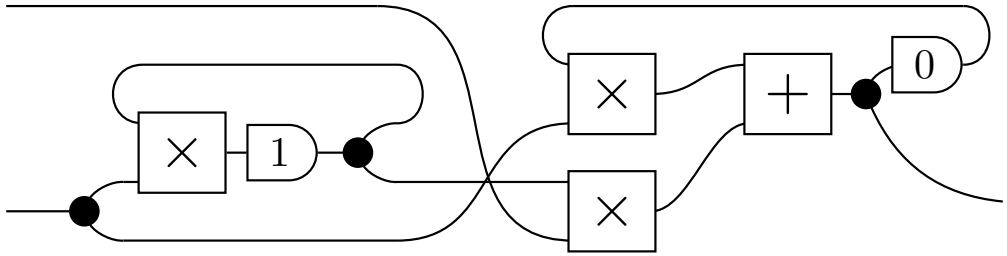
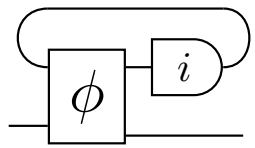


B. There is a general rule for derivatives of stateful functions



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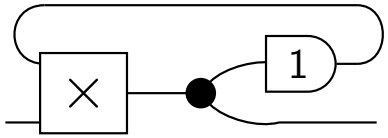
A. The derivative of 

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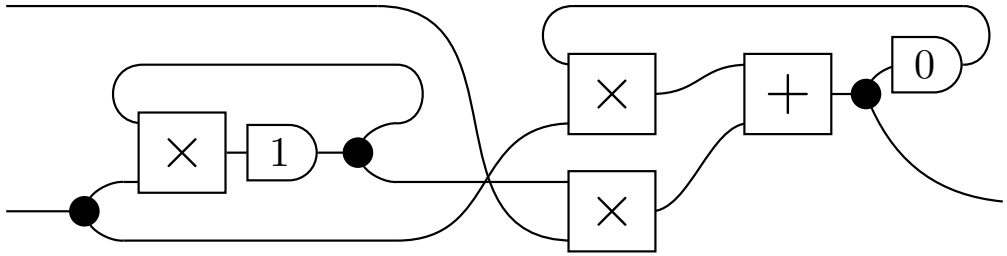

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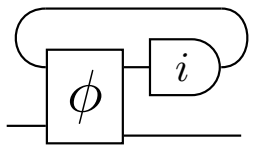

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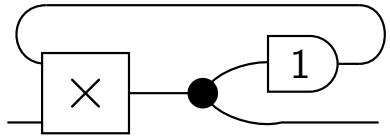
A. The derivative of 

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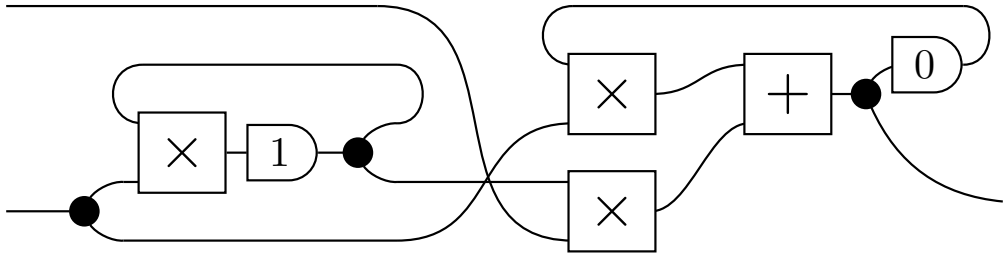

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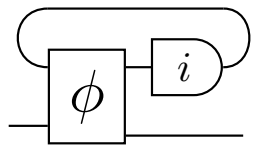

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⋮

Z. ~~Profit??~~ Get paper??

Goal Z & C: How do we get ¥¥¥?

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Answer: Use it for machine learning.

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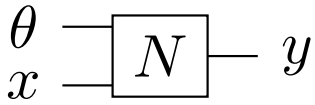
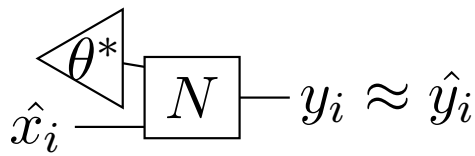
A *neural network* looks like 

. *Training* a neural network means finding θ^* so that:



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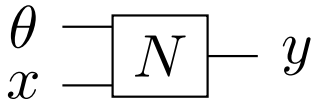
A *neural network* looks like 

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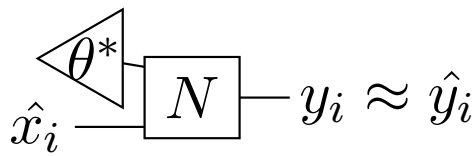

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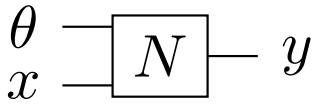
A *neural network* looks like 

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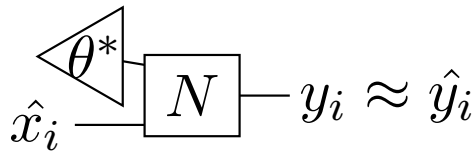

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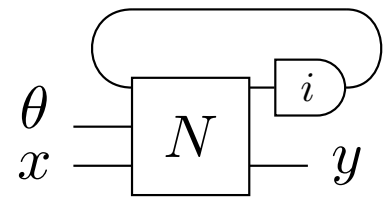
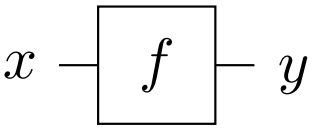
Upshot: If we can find (partial) derivatives of 

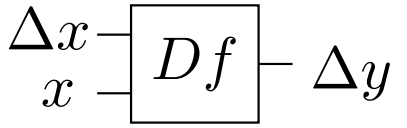
,
we can train recurrent neural networks. Using **properties** of these derivatives, maybe we can do it more efficiently than before.

Goal B: Derivatives in diagram form

The derivative of x — f — y is $\begin{matrix}\Delta x \\ x\end{matrix}$ — Df — Δy, which gives the best linear approximation to ϕ at a base point x.

Goal B: Derivatives in diagram form

The derivative of 

is 

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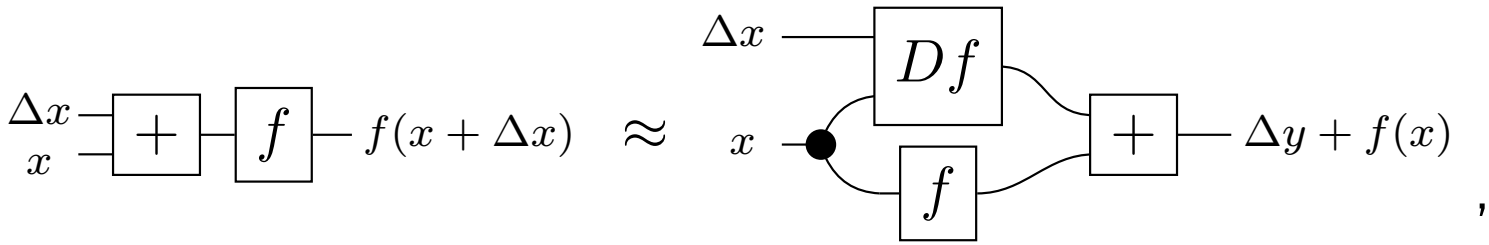
1. 

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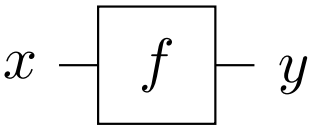
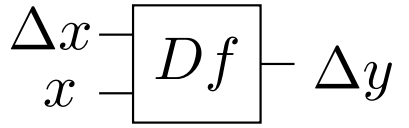
The derivative of 

is 

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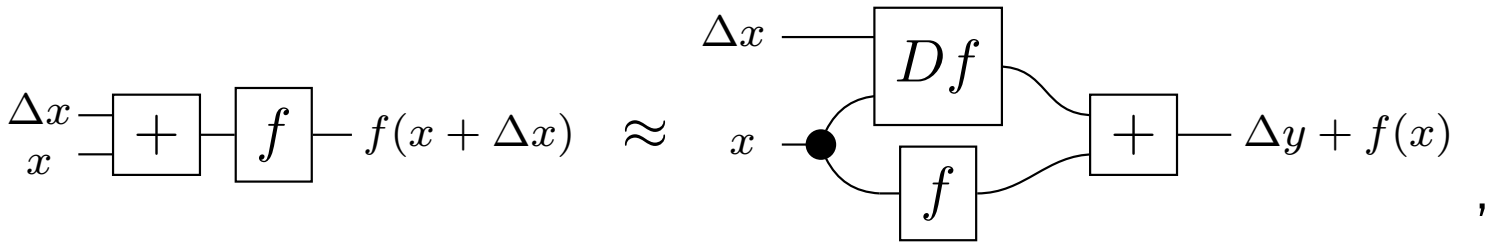
1. 

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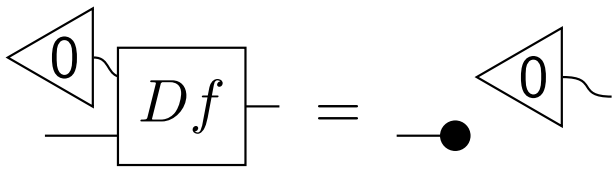
2. 

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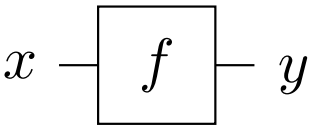
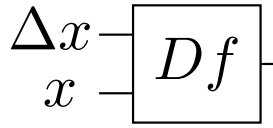
The derivative of 

is 

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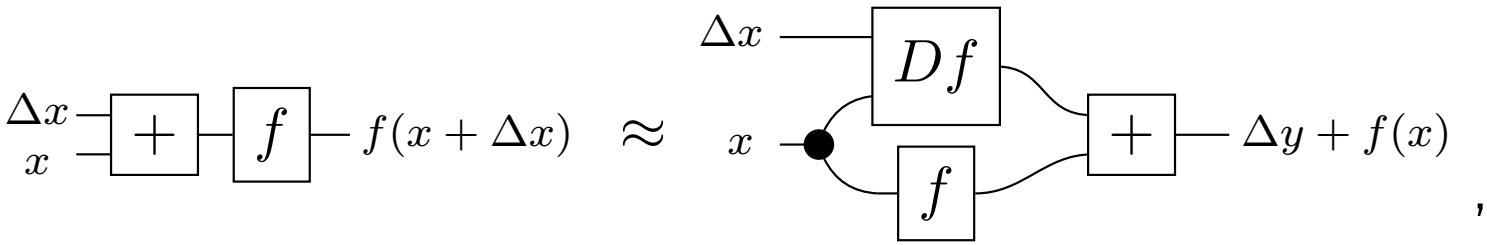
1. 

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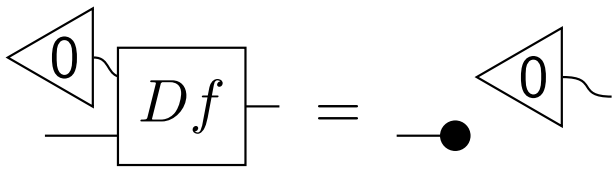
2. 

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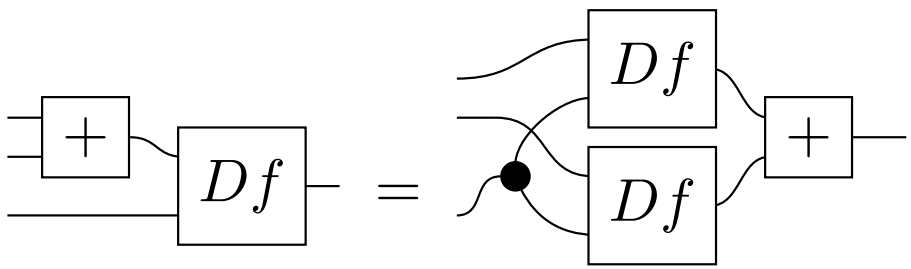
3. 

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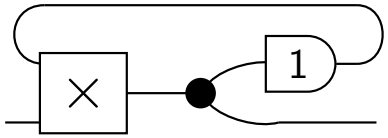
Goal A: Does the monster approximate output change?

Let $\Phi =$ 

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What is $D\Phi((0.1, 1), (0.1, 1), (0.1, 1), \ldots)$?

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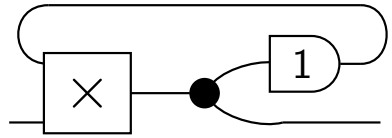
Let $\Phi =$ 

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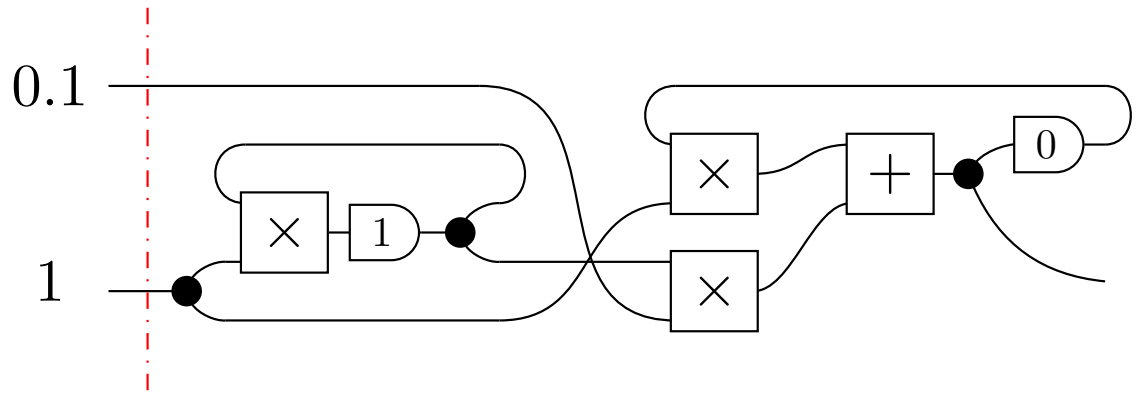

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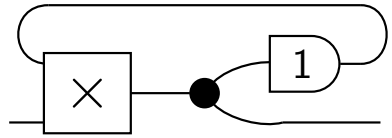
Let $\Phi =$ 

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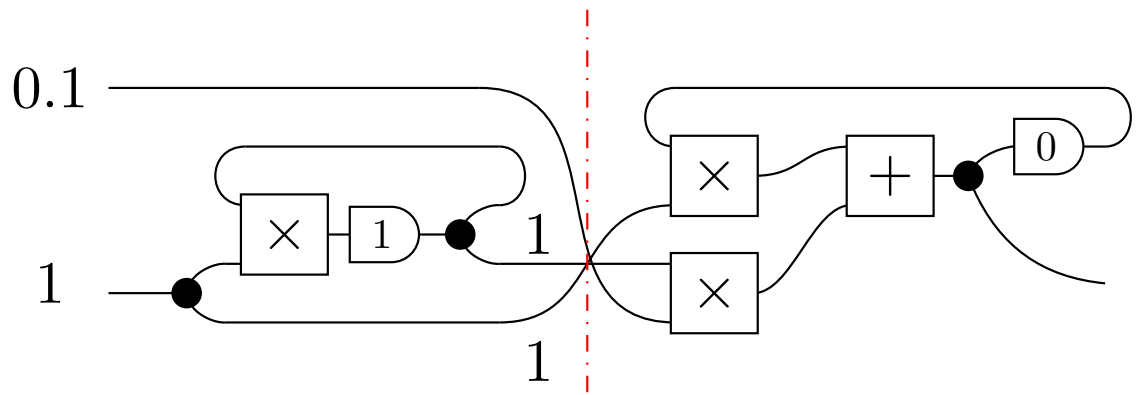

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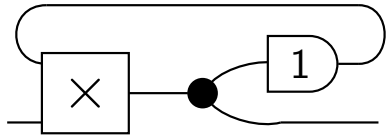
Let $\Phi =$ 

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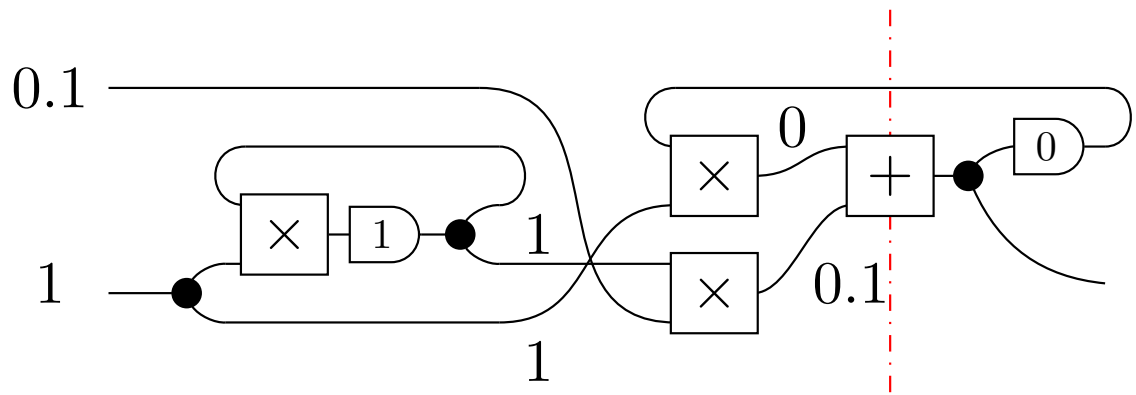

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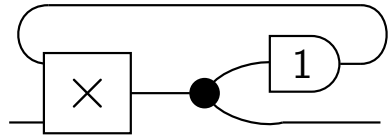
Let $\Phi =$ 

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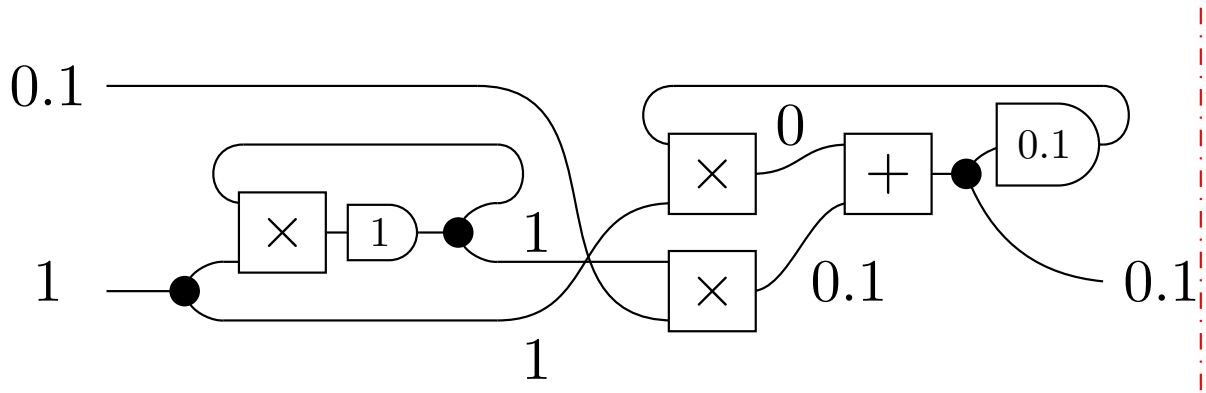

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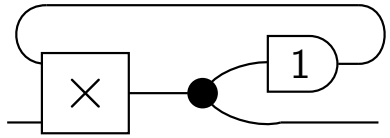
Let $\Phi =$ 

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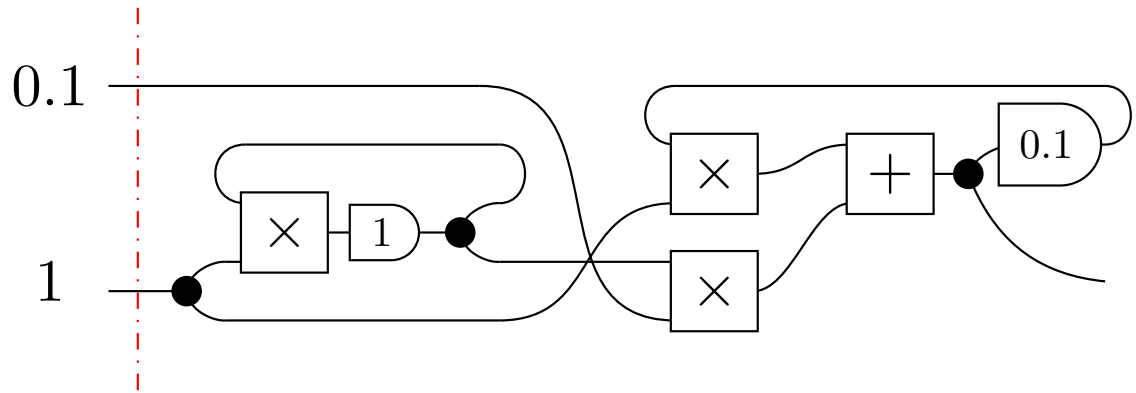

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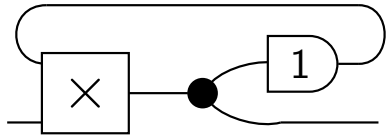
Let $\Phi =$ 

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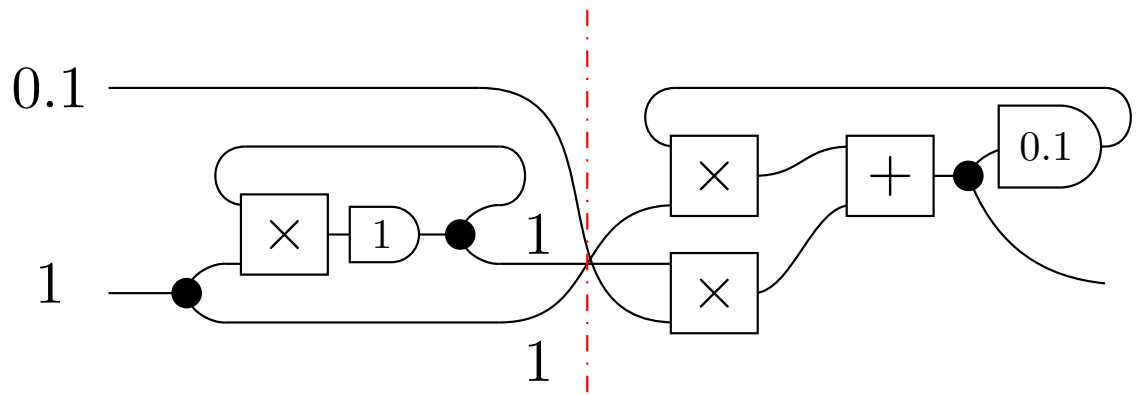

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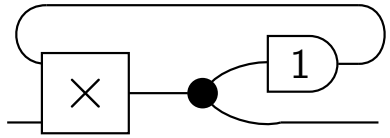
Let $\Phi =$ 

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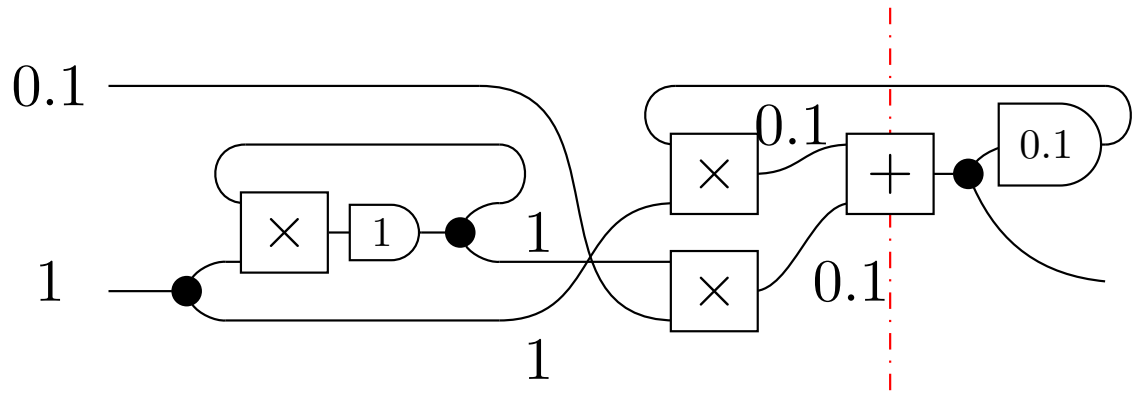

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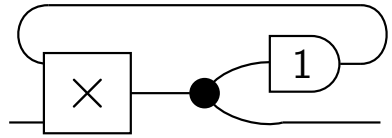
Let $\Phi =$ 

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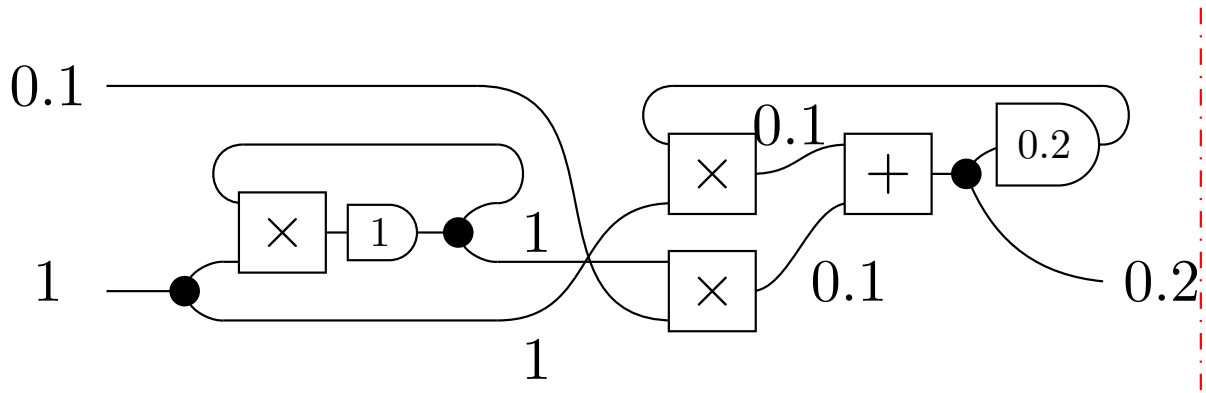

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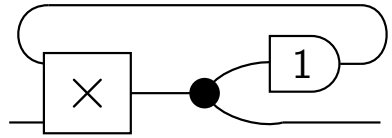
Let $\Phi =$ 

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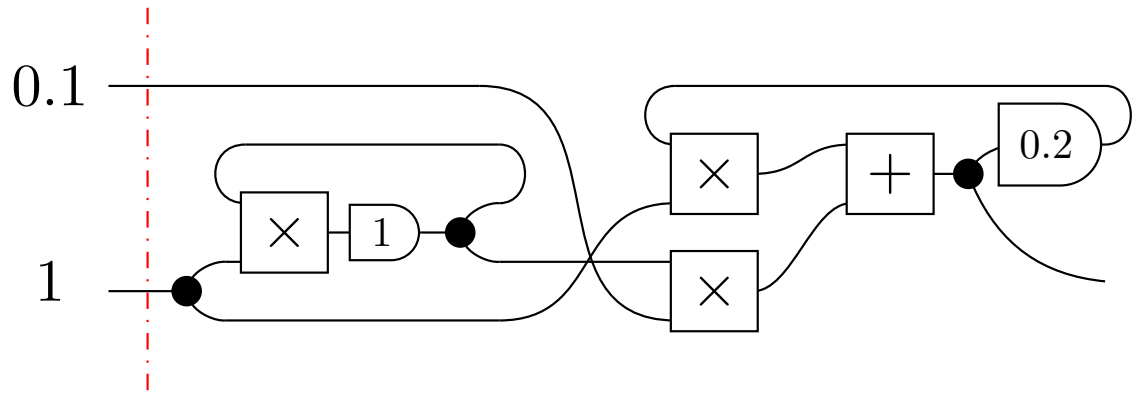

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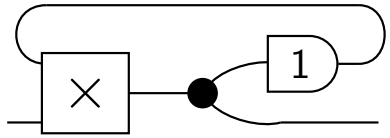
Let $\Phi =$ 

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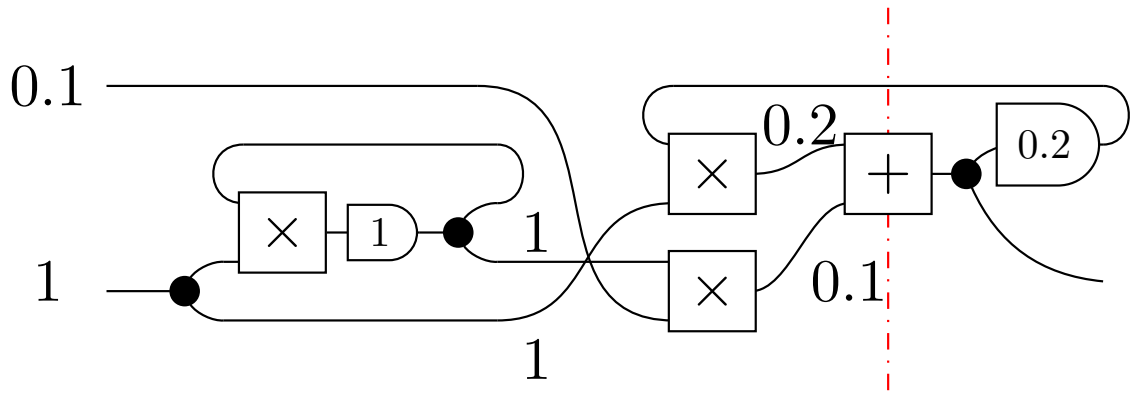

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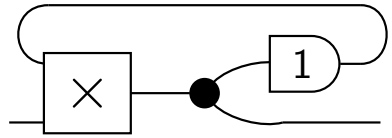
Let $\Phi =$ 

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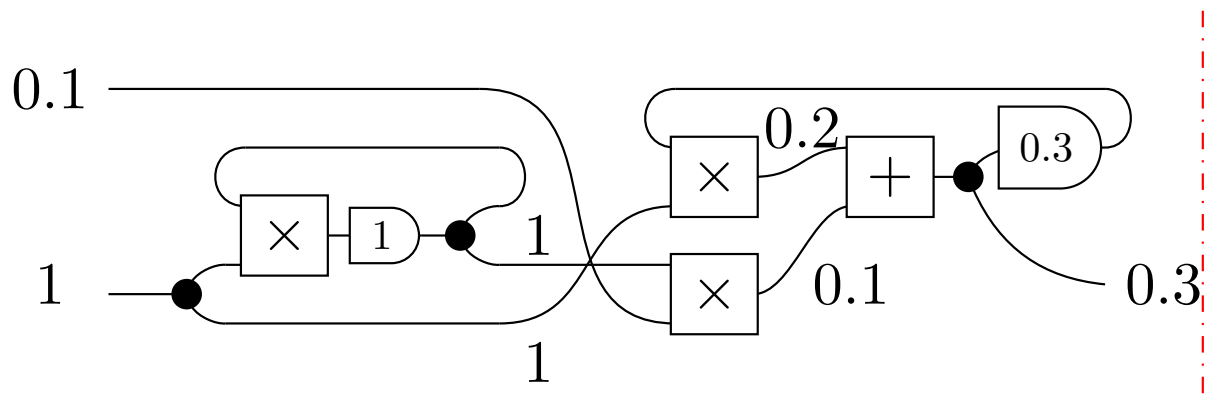

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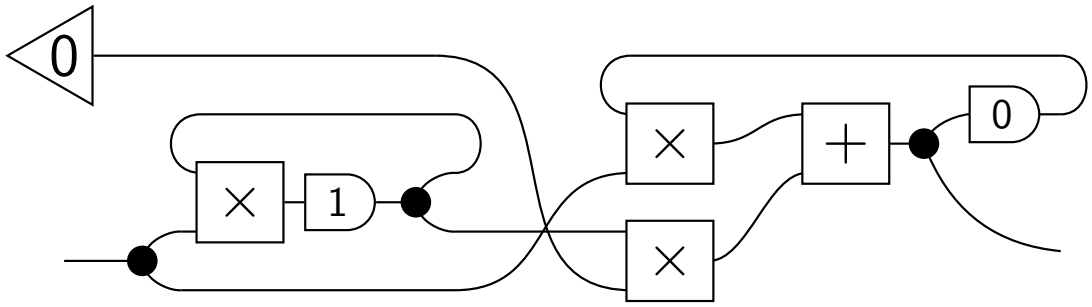

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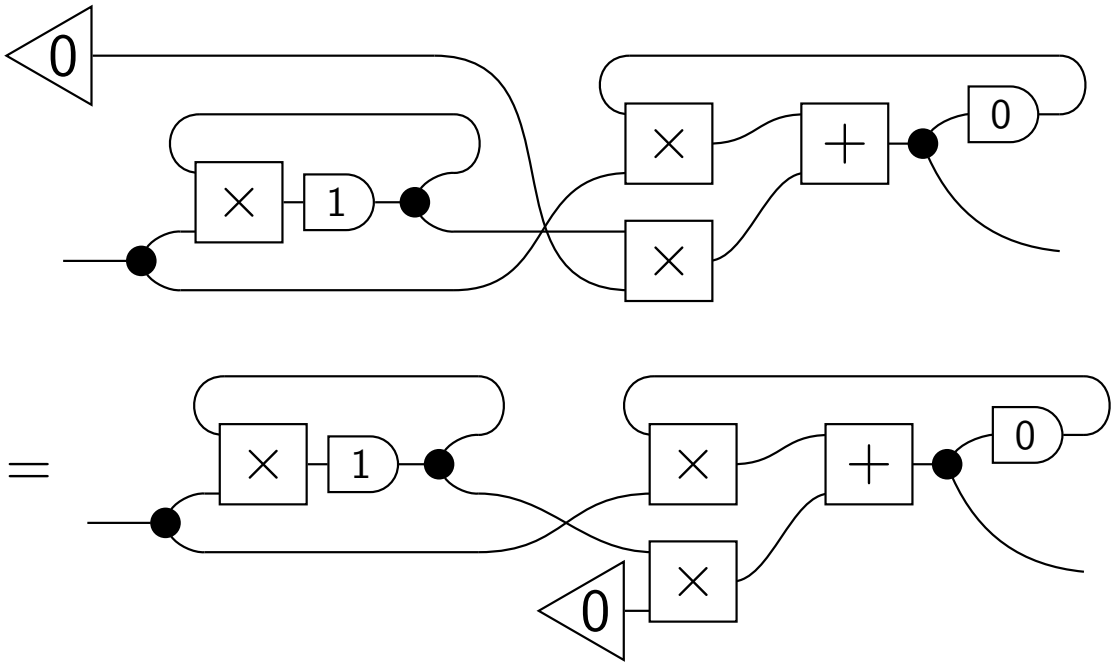

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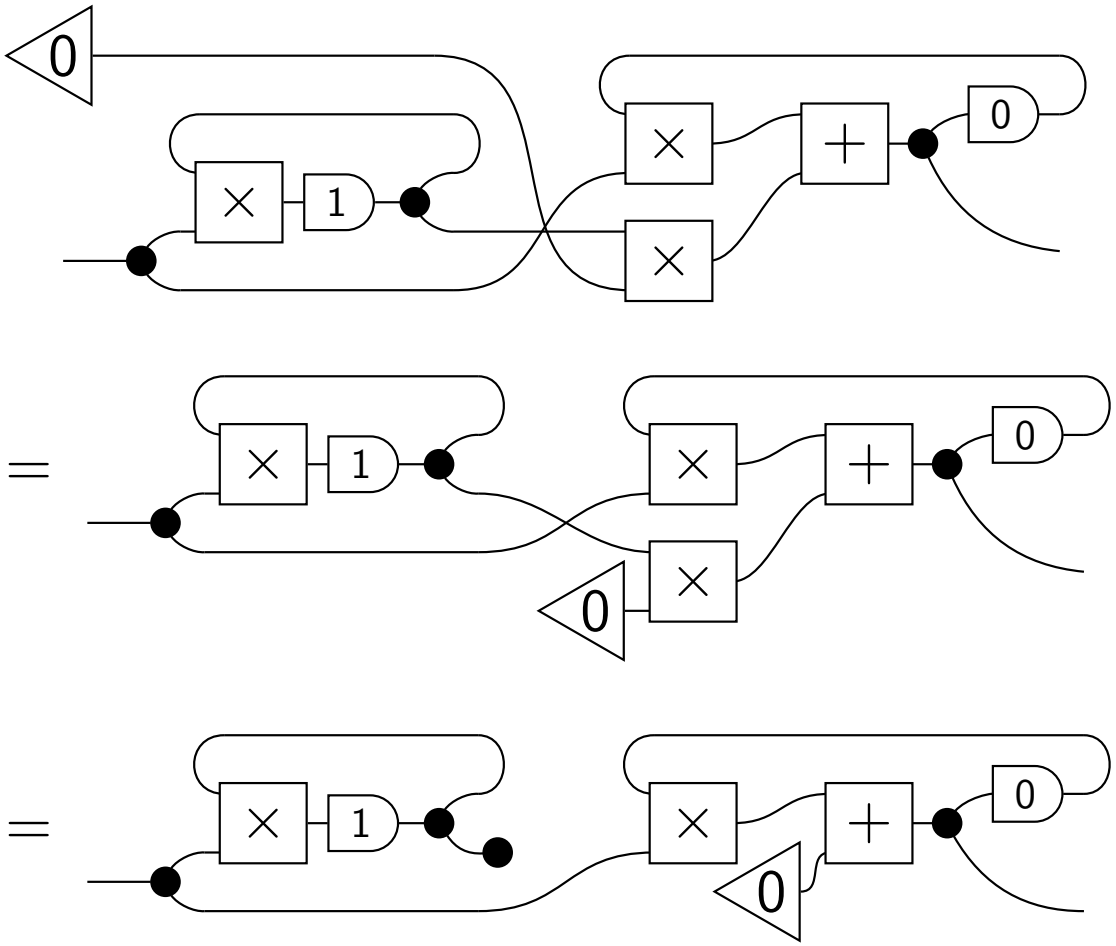

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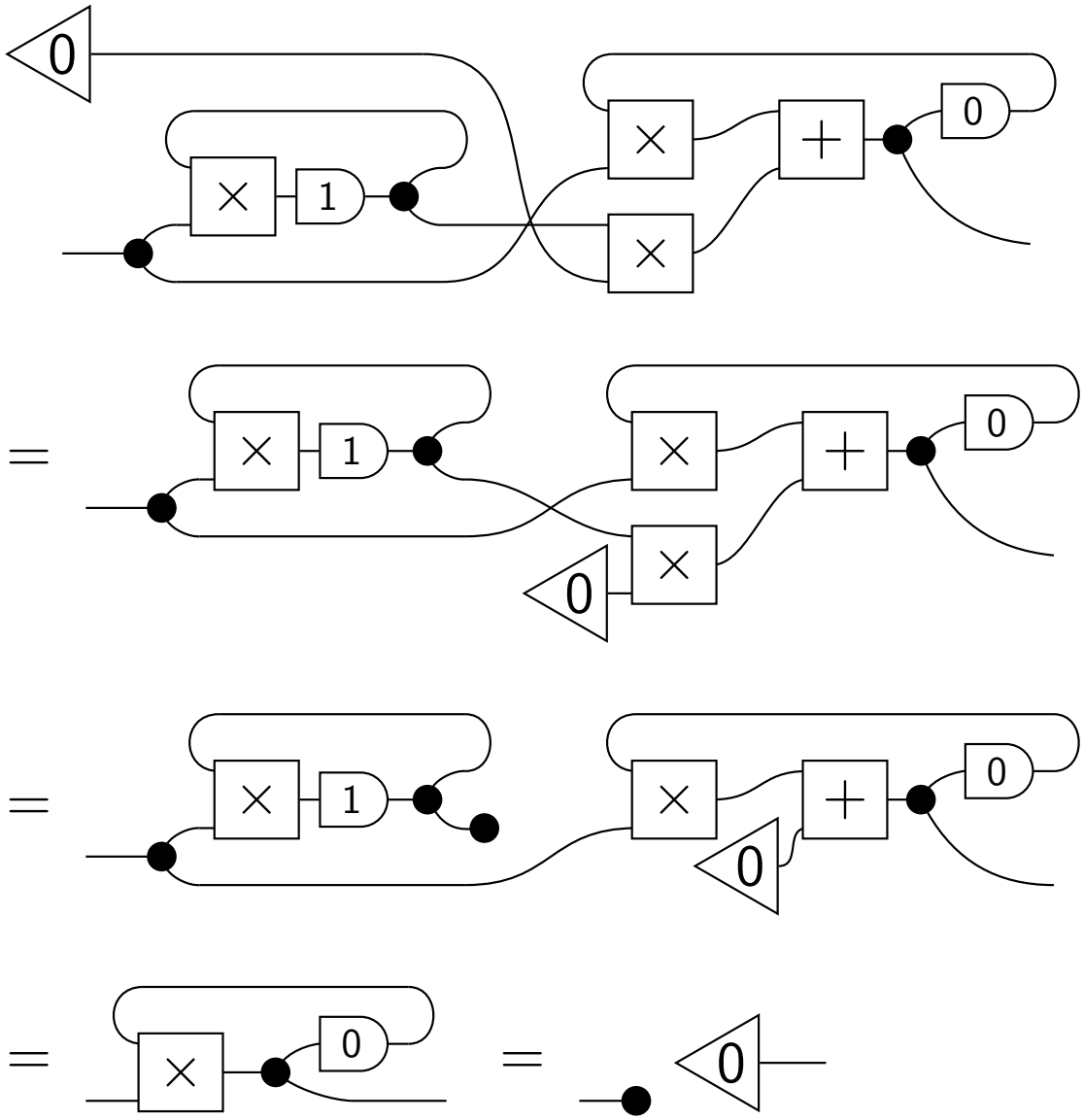

Outline

Main ideas

We imagine that we are starting from a (strictified Cartesian) category $\mathbb{C}$ whose morphisms represent single computations, which we aim to extend to computations on sequences.

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We want to capture *causal* functions on sequences, meaning the nth element of the output sequence depends only on the first n elements of the input sequence.

Main ideas

We imagine that we are starting from a (strictified Cartesian) category $\mathbb{C}$ whose morphisms represent single computations, which we aim to extend to computations on sequences.

We want to capture *causal* functions on sequences, meaning the nth element of the output sequence depends only on the first n elements of the input sequence.

There are three steps:

1. describe a single step of the sequence computation, including a mechanism for sending and receiving state,
2. chain these single steps together to get a full sequence, and
3. quotient these computations by their observable behaviour.

Step 1: Single computation steps

We separate inputs and outputs of a $\mathbb{C}$-morphism into two types: *values*, exchanged with the environment, and *states*, received from (sent to) the previous (next) step of the computation.

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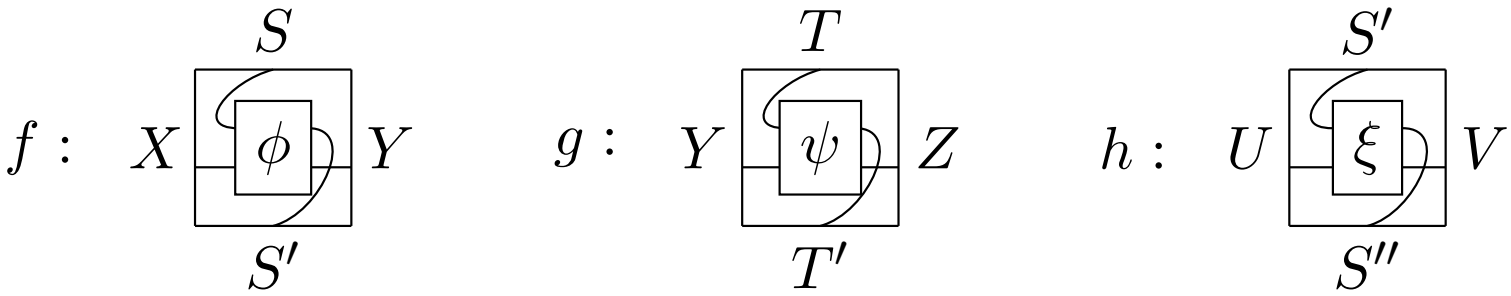
Definition

A *computation step* $f : X \xrightarrow[S']{S} Y$ is four objects and a morphism:

1. S — the input state received from the previous step
2. X — the input value received from the environment
3. S' — the output state sent to the next step
4. Y — the output value sent to the environment
5. $\phi : S \times X \to S' \times Y$ — the $\mathbb{C}$-morphism doing the computation

Step 1: Single computation steps

We can draw a single step like so:



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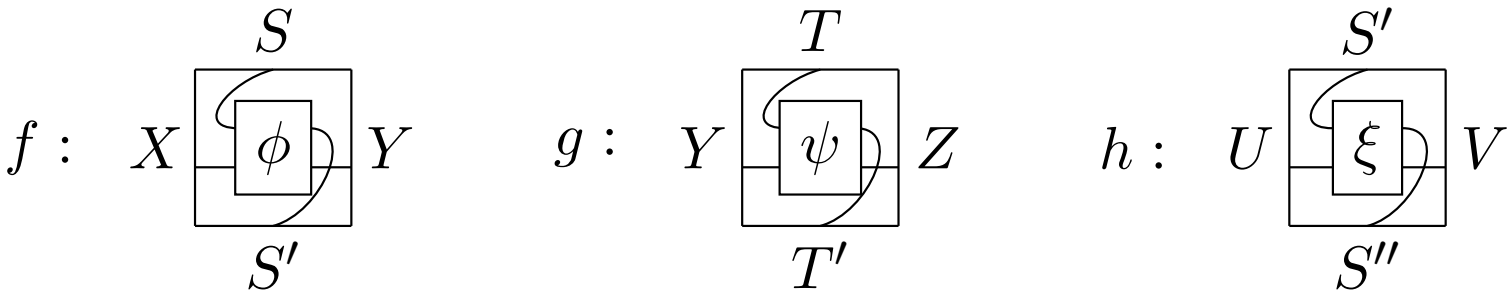
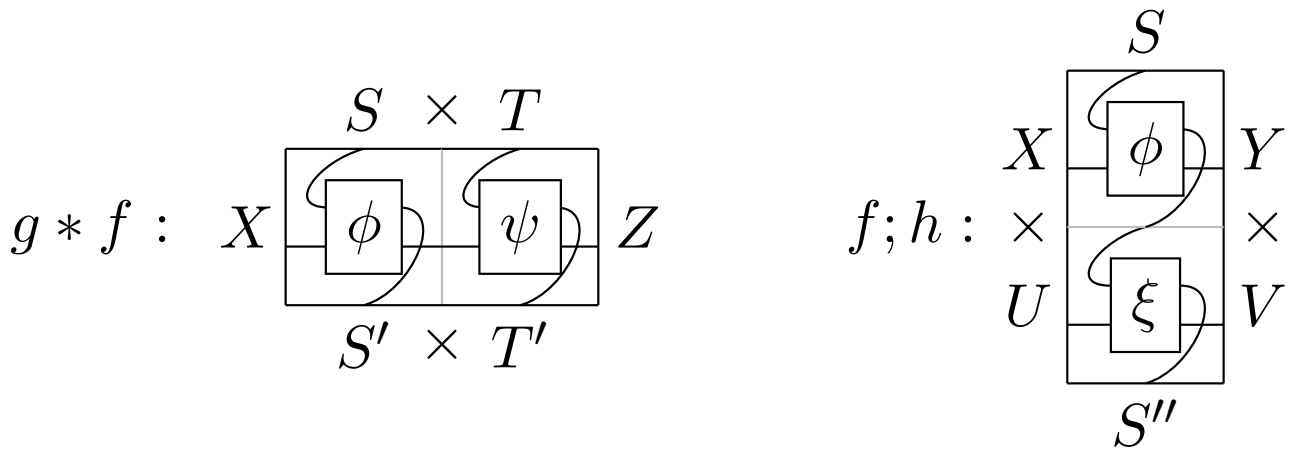


Computation steps can be composed in two different ways:



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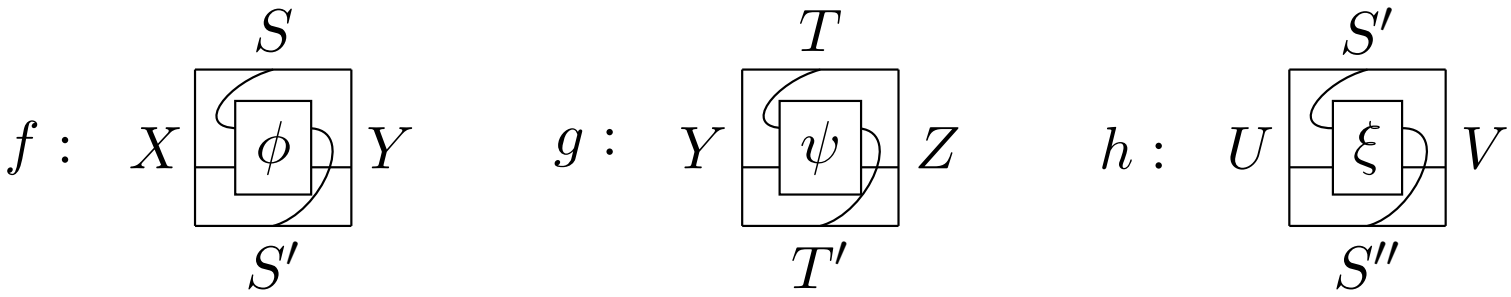

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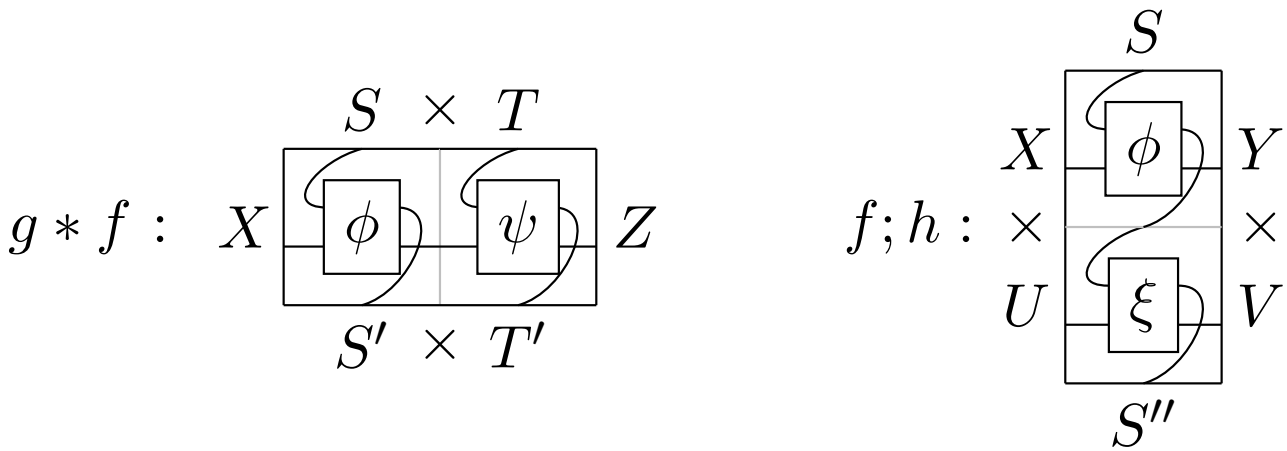


psst . . . double category

Step 2: Computation sequences

Next, we chain together infinitely many of these computation steps to compute a whole sequence of outputs.

Definition

A *computation sequence* $\mathbf{f} = (i, [f_k])$ is an infinite sequence of computation steps $f_k : X_k \xrightarrow[S_{k+1}]{S_k} Y_k$, and an initial state $i : 1 \xrightarrow[S_0]{1} 1$. We say $\mathbf{f}$ takes sequences of type $[X_k] = (X_0, X_1, \ldots, X_n, \ldots)$ to sequences of type $[Y_k] = (Y_0, Y_1, \ldots, Y_n, \ldots)$.

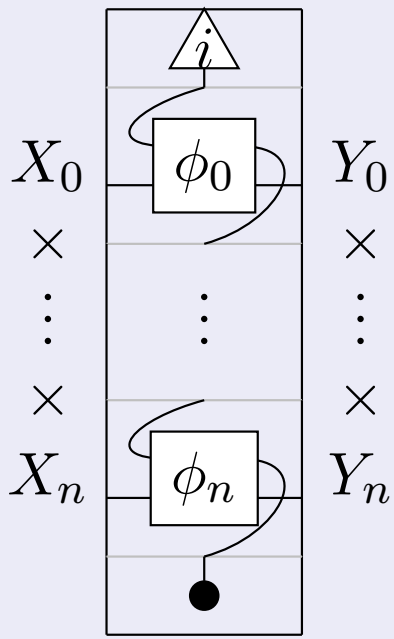
Note that f_k and f_{k+1} are vertically composable, as are i and f_0.

Step 3: Comparing computation sequences

Two computation sequences might have different state spaces and still compute the same function. We need to make some identifications. . .

Definition

The n*th truncation* of a computation sequence is the morphism of the vertical composite of the first $n+1$ steps:



Step 3: Comparing computation sequences

Definition

Two computation sequences $\mathbf{f}, \mathbf{g} : [X_k] \to [Y_k]$ are *extensionally equivalent* means they have the same nth truncation for all $n \in \mathbb{N}$.

Definition

A *stateful (sequence) function* is an extensional equivalence class of computation sequences.

Definition

If $\mathbb{C}$ is a (strict) Cartesian category, then its *stateful extension* is a category $\mathrm{St}(\mathbb{C})$ where

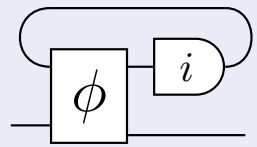
- objects are $[X_k]$, i.e. infinite sequences of objects in $\mathbb{C}$ and
- morphisms are stateful functions $\mathbf{f} : [X_k] \to [Y_k]$.

Sanity checks

Theorem

The homset $\mathrm{St}(Set)([A],[B])$ *is in 1-1 correspondence with the set of causal functions from* A^ω *to* B^ω*.*

Theorem

The sequence of n*th truncations of* $(i,[\phi])$*, each projected to their last component, is the unrolling of* 

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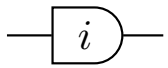
Fill-in-the-blank

How would you implement 

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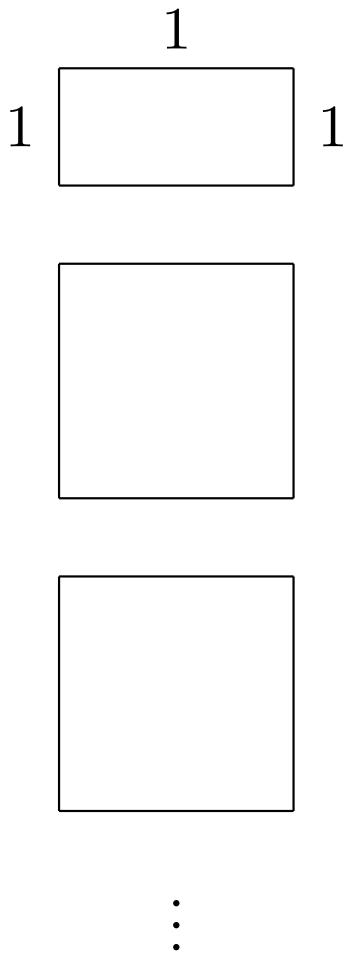

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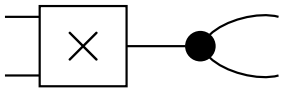
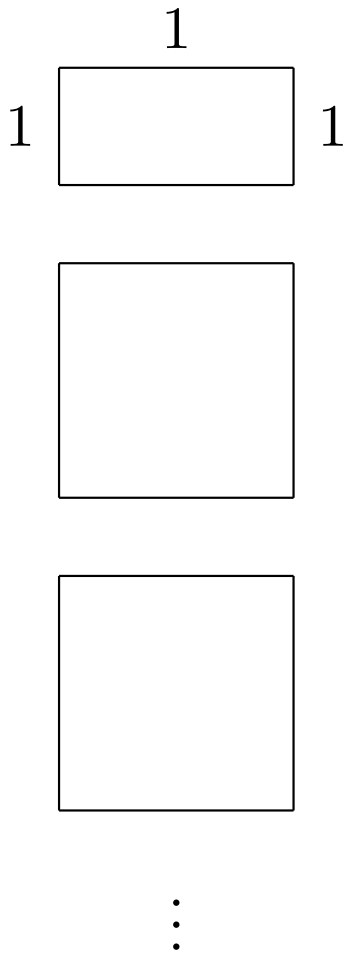
How would you implement  as a computation sequence?



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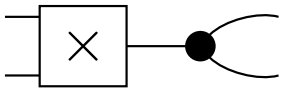
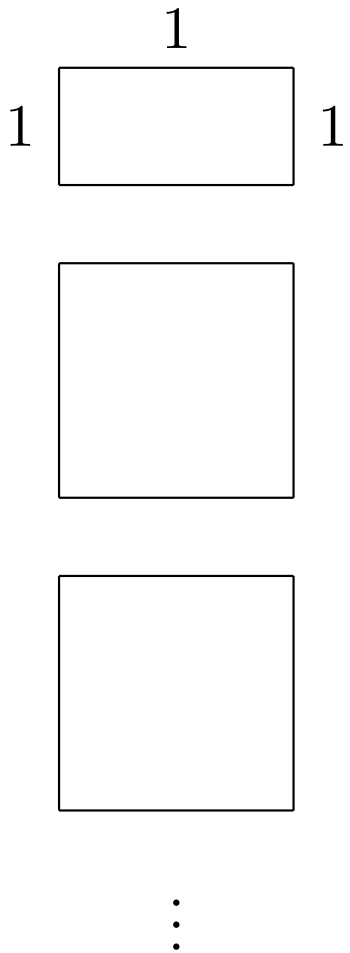
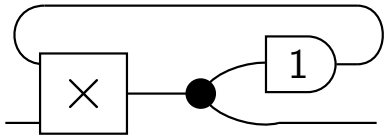
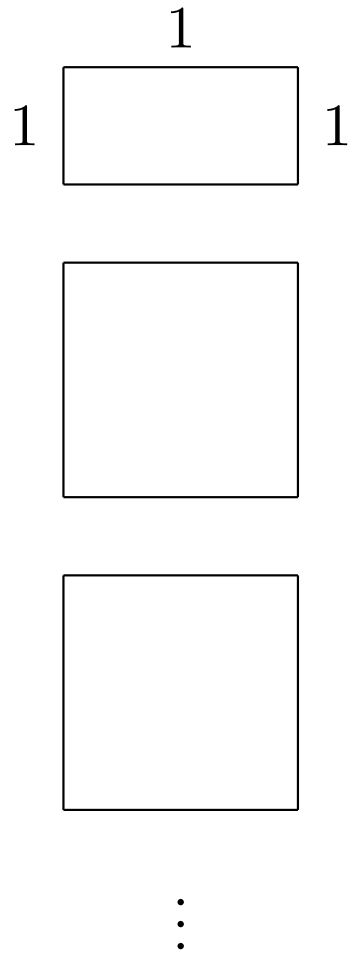
How would you implement  as a computation sequence?



How would you implement  as a computation sequence?

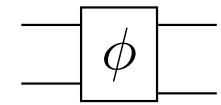


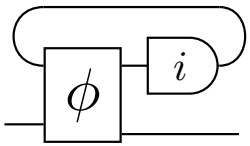
Outline

Delayed trace

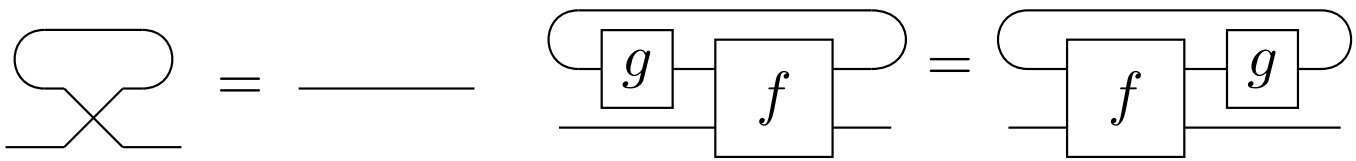
This loop-with-delay-gate is a trace-like operation.

$$\frac{\phi : S \times X \to S \times Y}{dtr_i^S(\phi) : X \to Y}$$

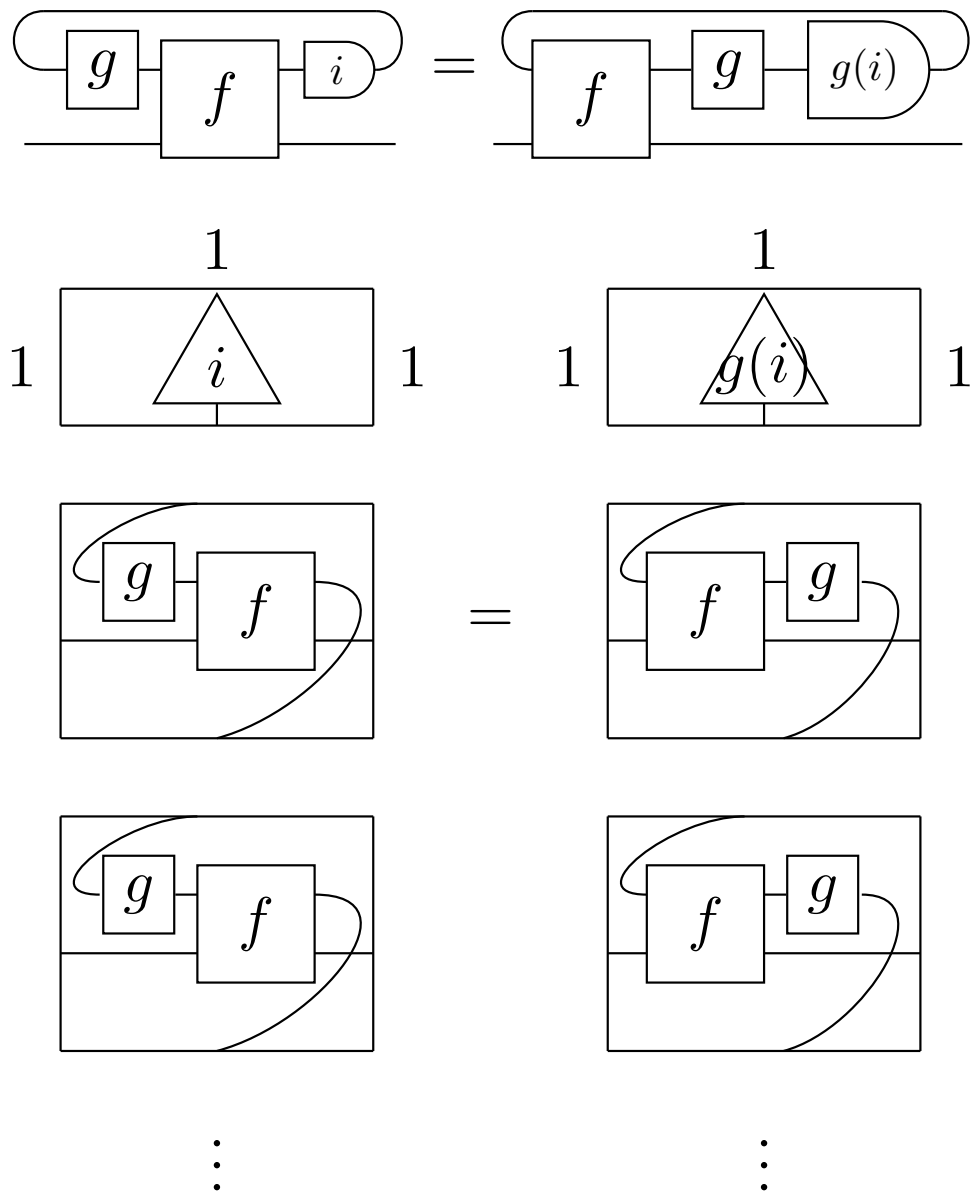




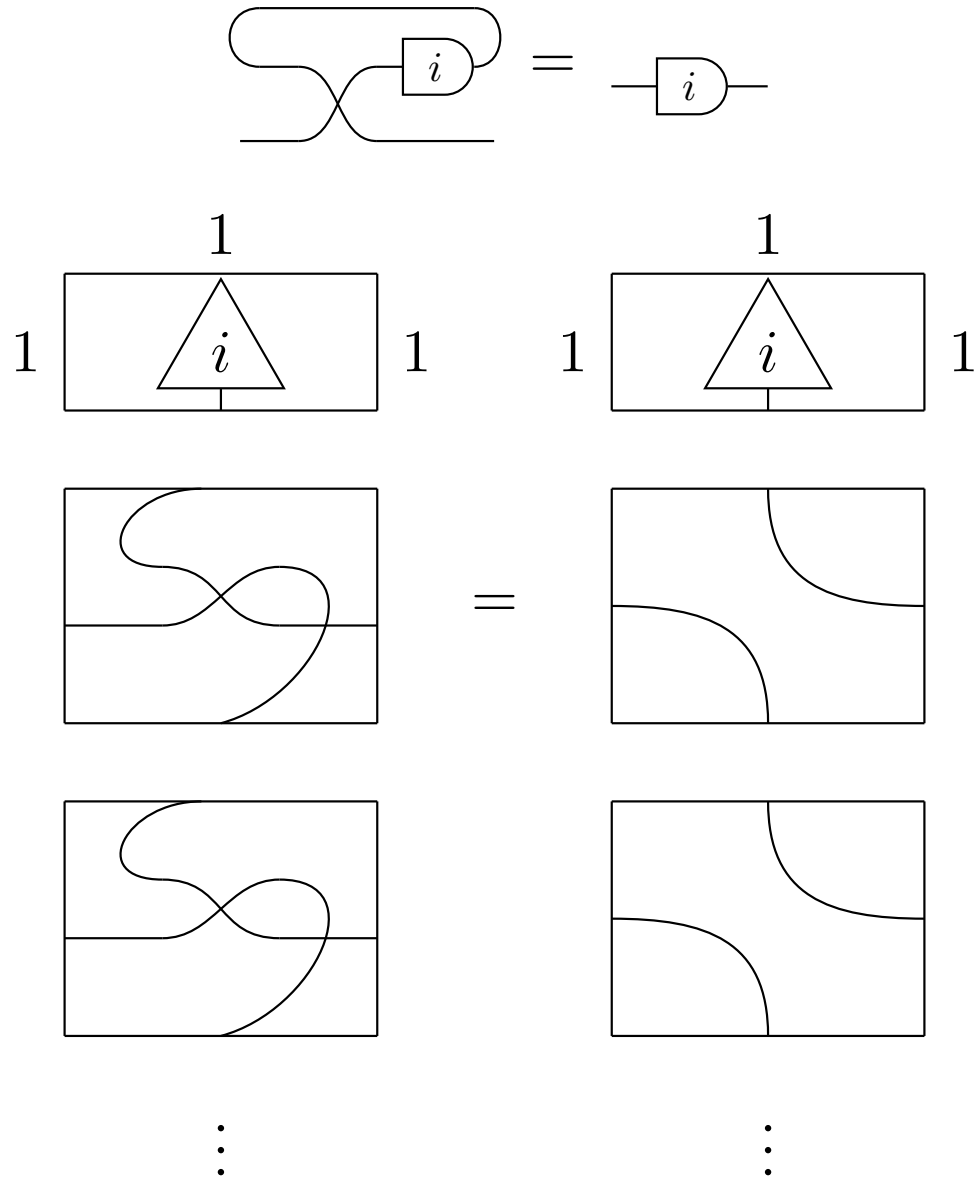
It satisfies **most** of the the trace axioms (source & target naturality, vanishing 1 and $\times$, and superposing) but misses two: yanking and dinaturality. For regular trace, those are



~~Dinaturality~~ → retiming



~~Yanking~~ → delay



Advantages of delayed trace

Often, people formalizing circuits in category theory do these:

1. (freely) add registers to the category,
2. add trace to the category,
3. restrict to a subcategory such that all traces are taken on positions guarded by a register.

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This ensures all loops are guarded (without a syntactic restriction!) and requires less structure.

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We are also interested in looking at delayed traces abstractly...

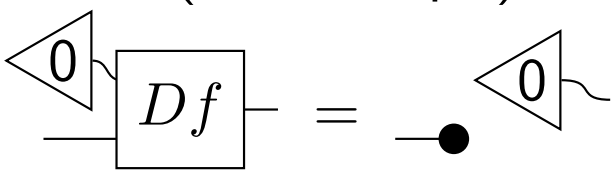
Outline

Cartesian differential categories [Blute, Cockett, Seely '09]

A *Cartesian differential category* has a differential operation on morphisms sending $f : X \to Y$ to $Df : X \times X \to Y$, satisfying:

CD1. $Ds = s \times !_{\mathrm{dom}(s)}$ for $s \in \{\mathrm{id}_X, \sigma_{X,Y}, !_X, \Delta_X, 0_X, +_X\}$.

CD2. (linear map I)



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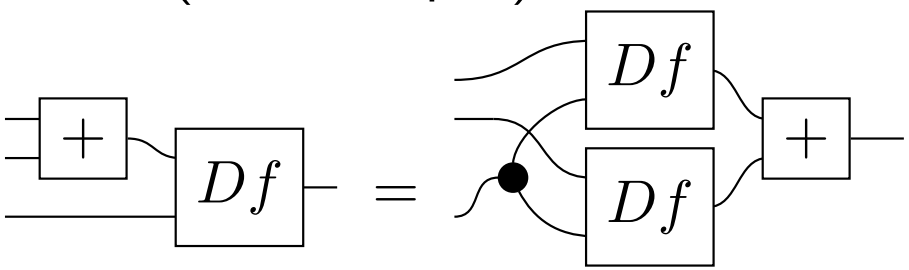
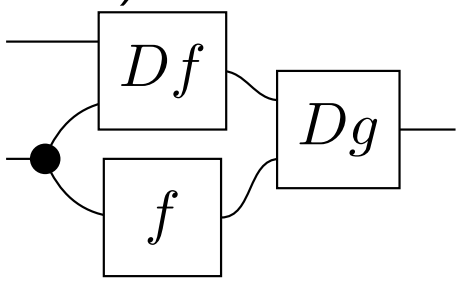


CD4. (chain rule)

$D(g \circ f) =$



CD5. (parallel rule)

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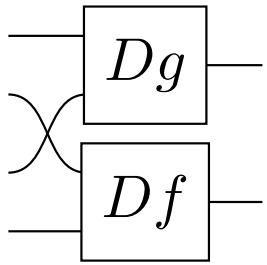

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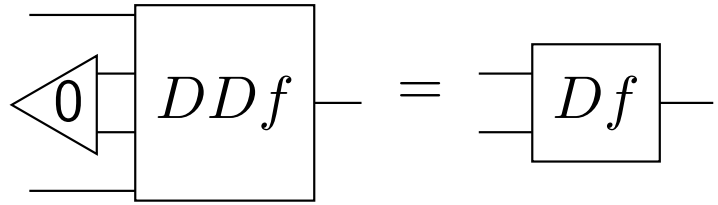
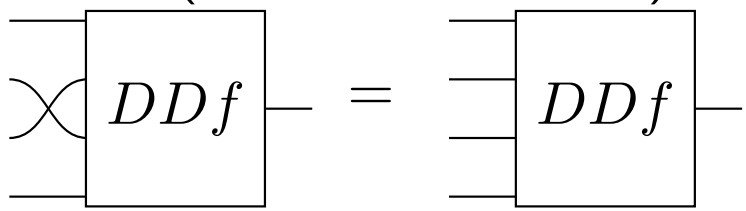


CD7. (Schwartz theorem)



$\mathbf{Euc}_\infty$ is Cartesian differential

The differential operator on Euclidean spaces and smooth maps sends $f : \mathbb{R}^n \to \mathbb{R}^m$ to $Df : (\Delta x, x) \mapsto Jf|_x \times \Delta x$.

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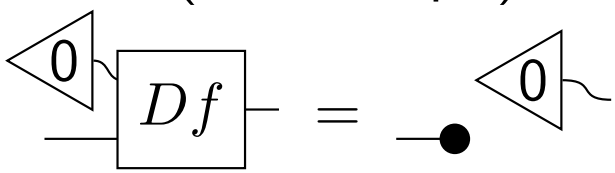

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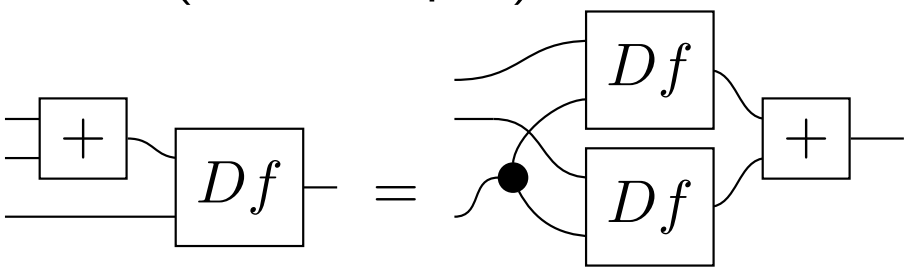

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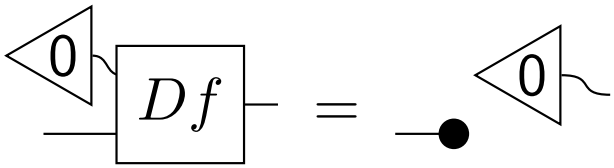

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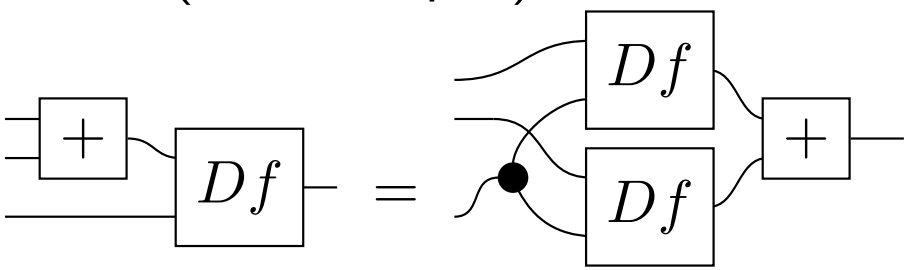

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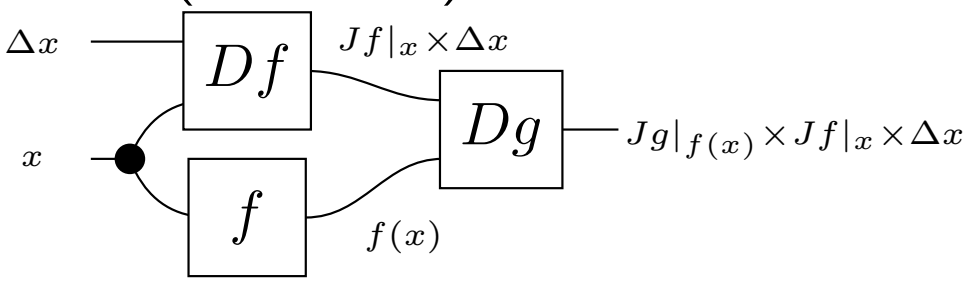

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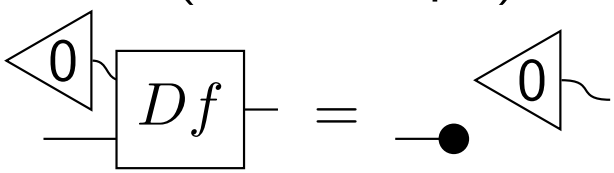

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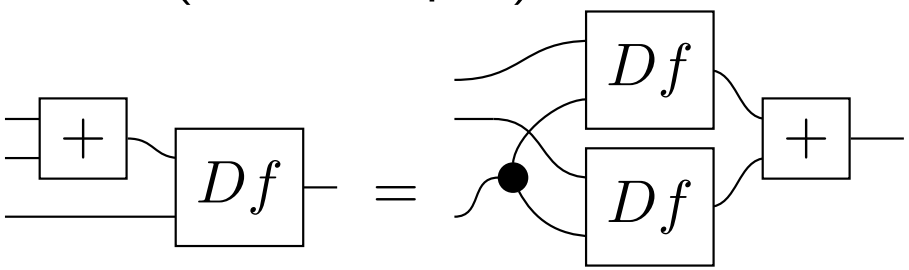

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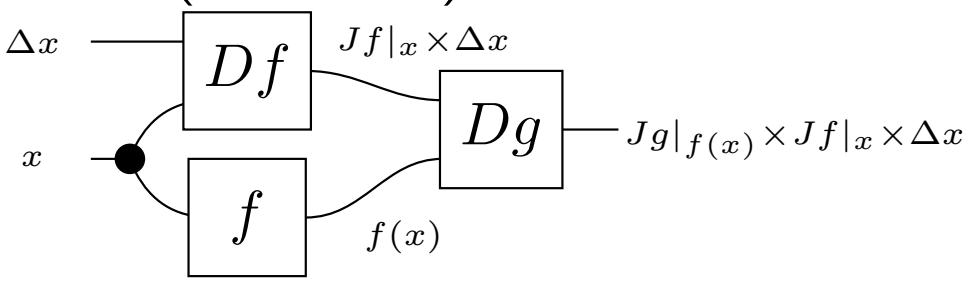

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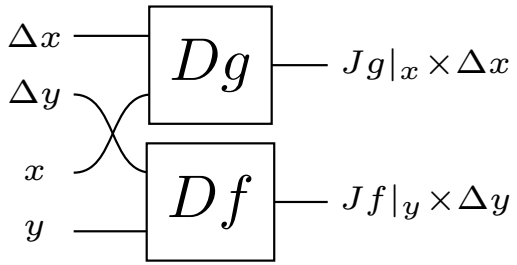

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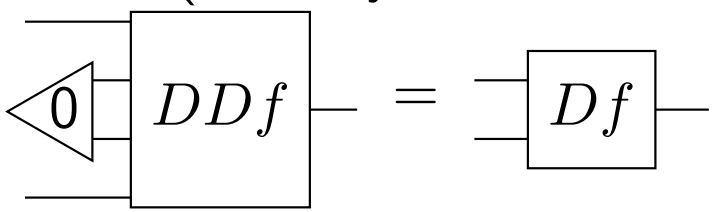

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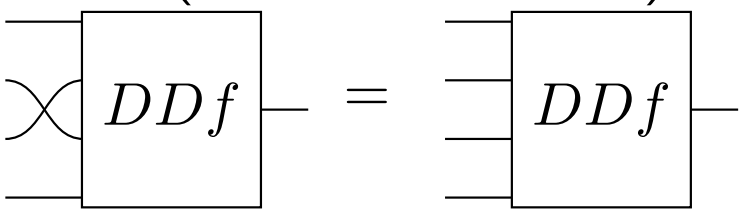
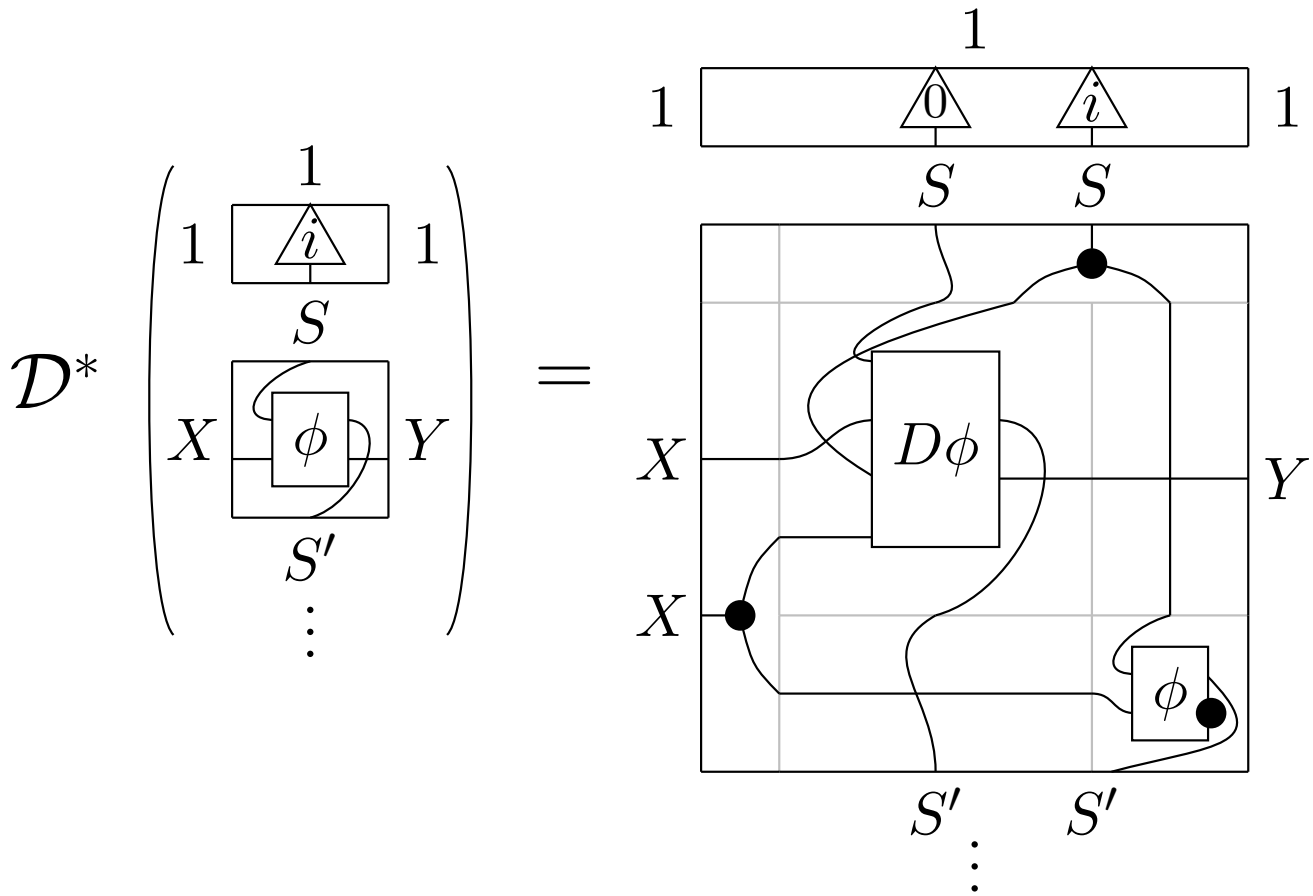


Key contribution: differential operator lifts

Theorem

If $\mathbb{C}$ is a Cartesian differential category, so is $\mathrm{St}(\mathbb{C})$.

The Cartesian differential operator on $\mathrm{St}(\mathbb{C})$ is defined as follows:



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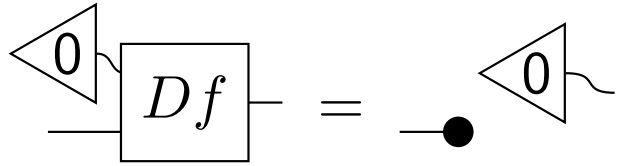
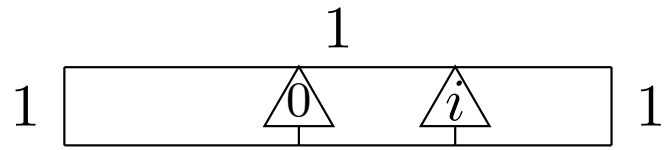
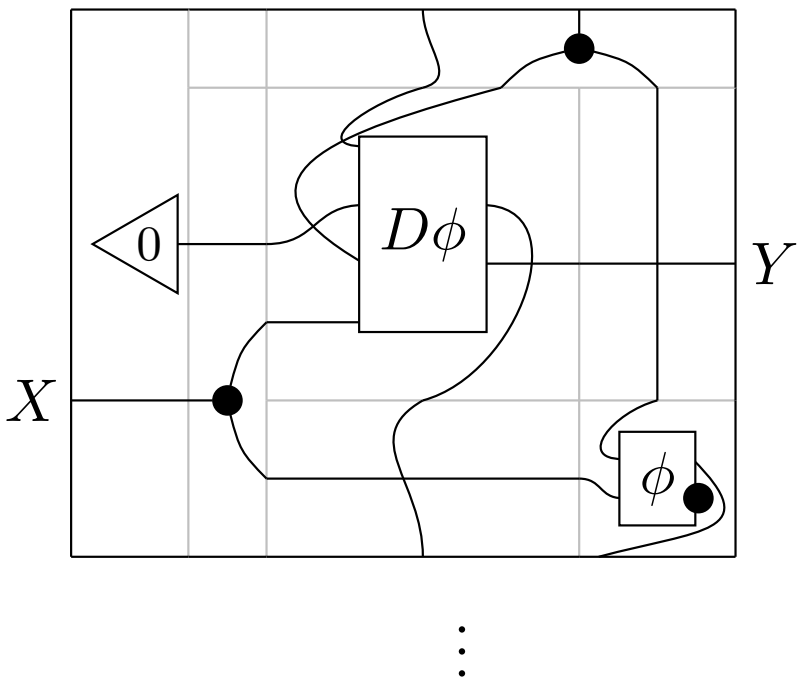
Proof idea. For CD2:







Key contribution: differential operator lifts

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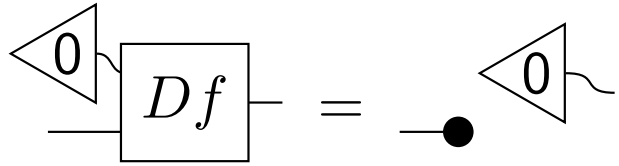

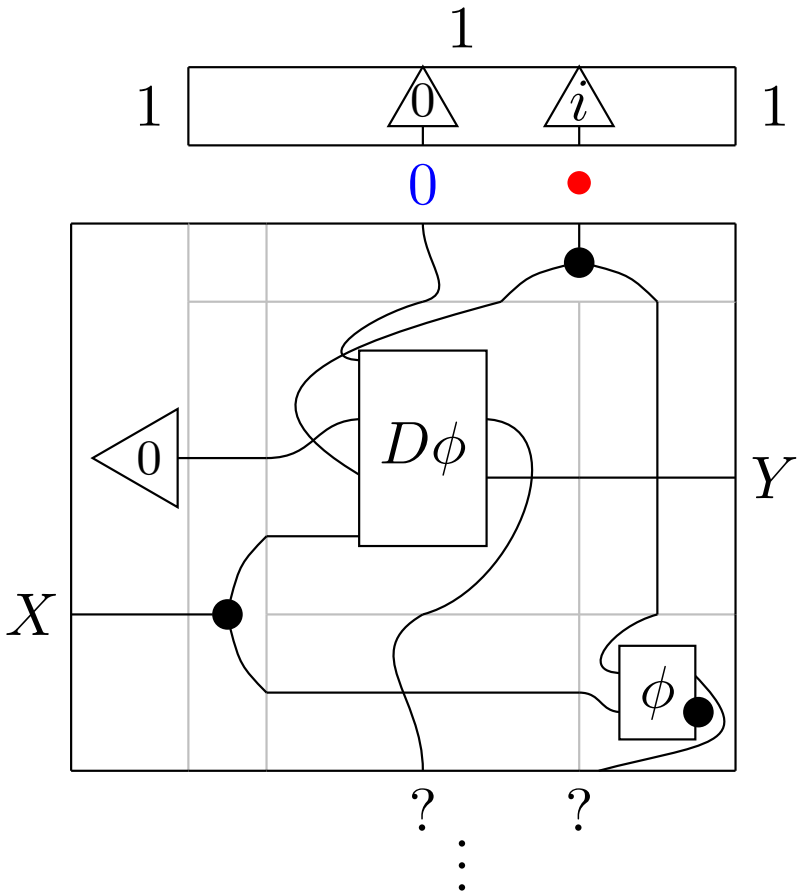

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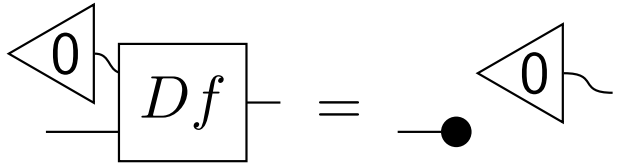

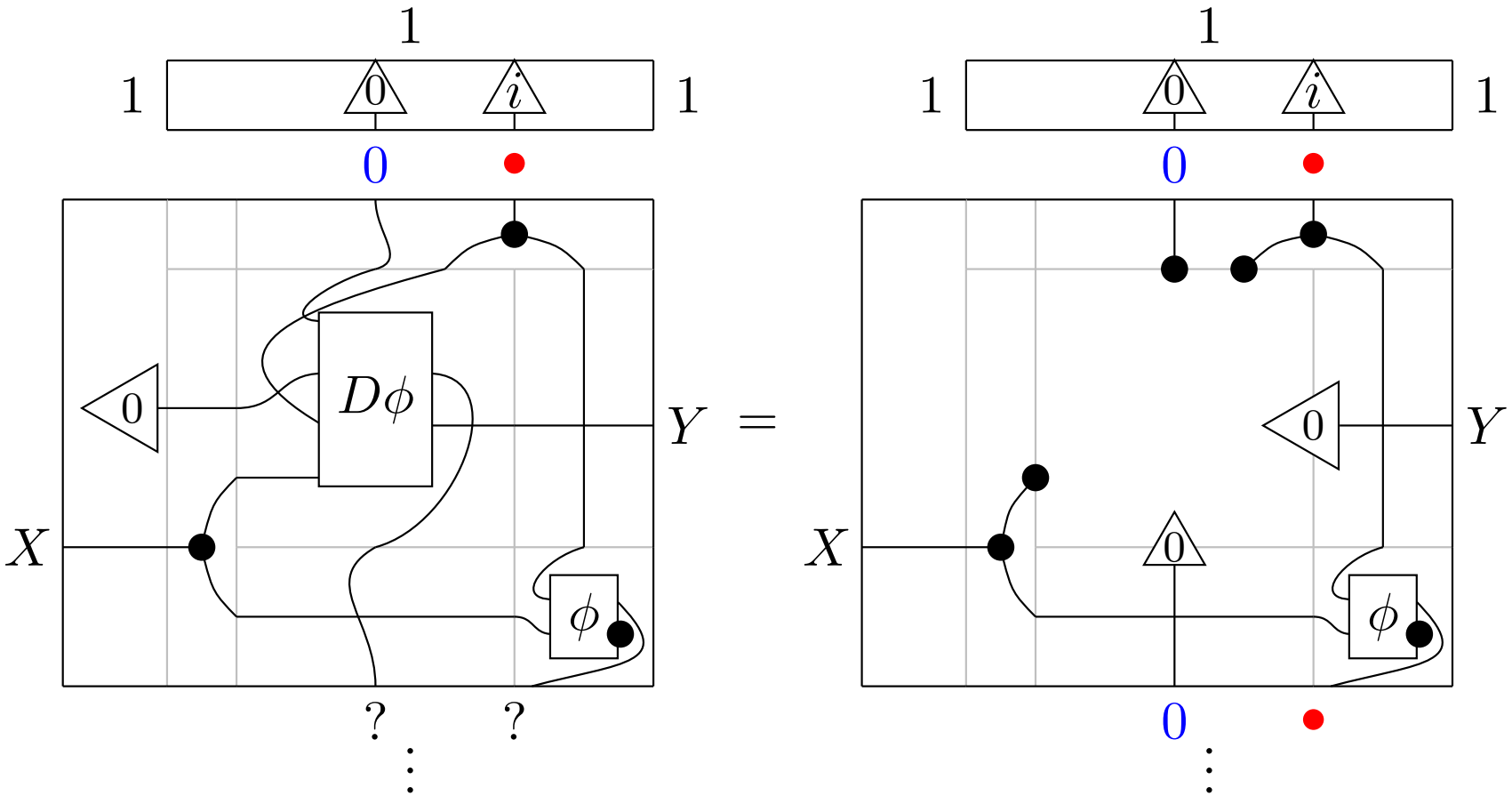

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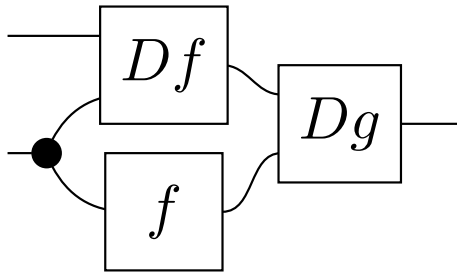
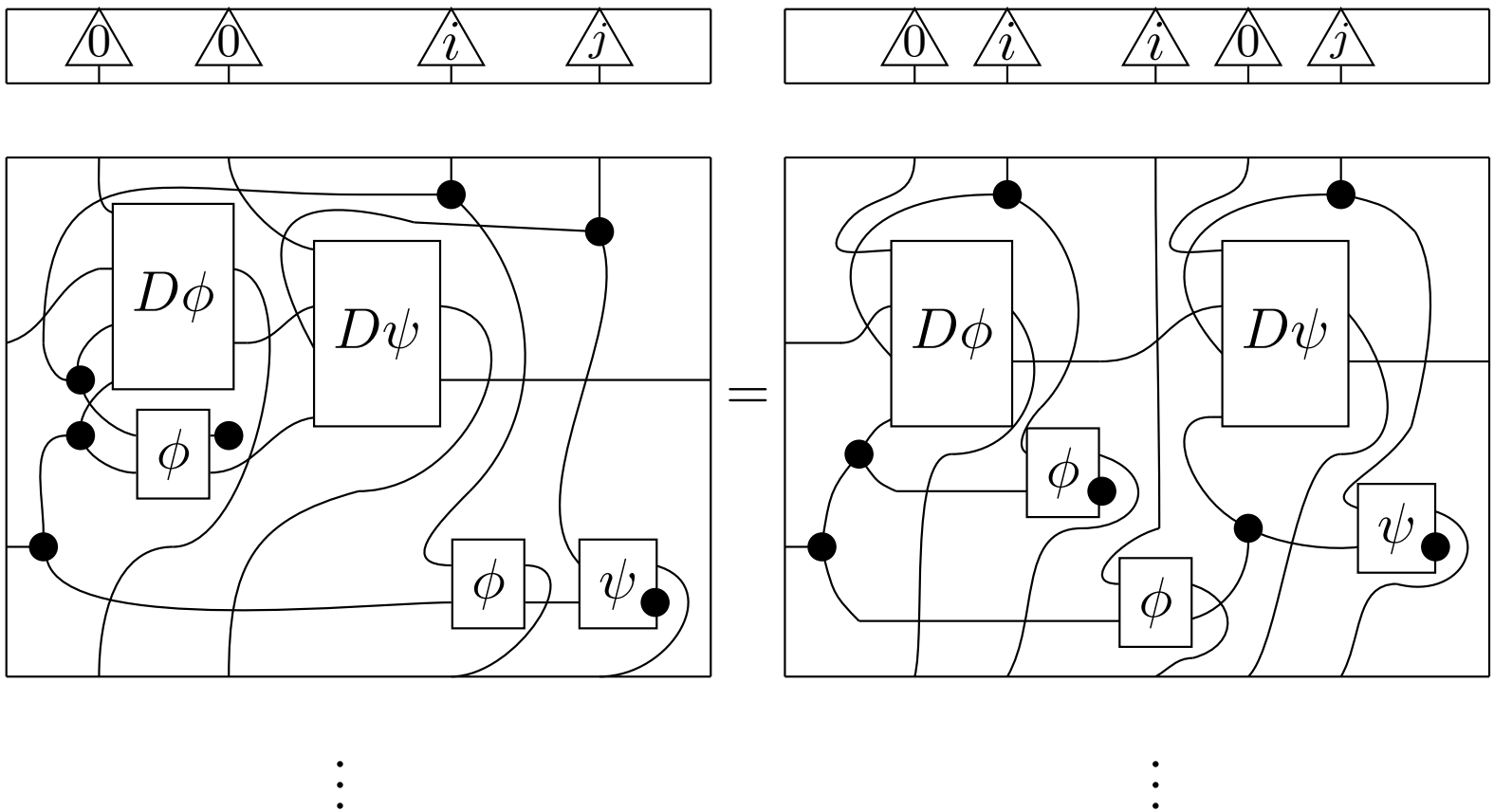
Proof idea. For CD4: $D(g \circ f) =$





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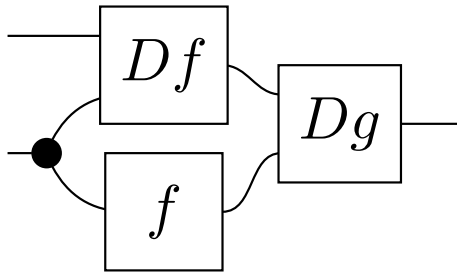

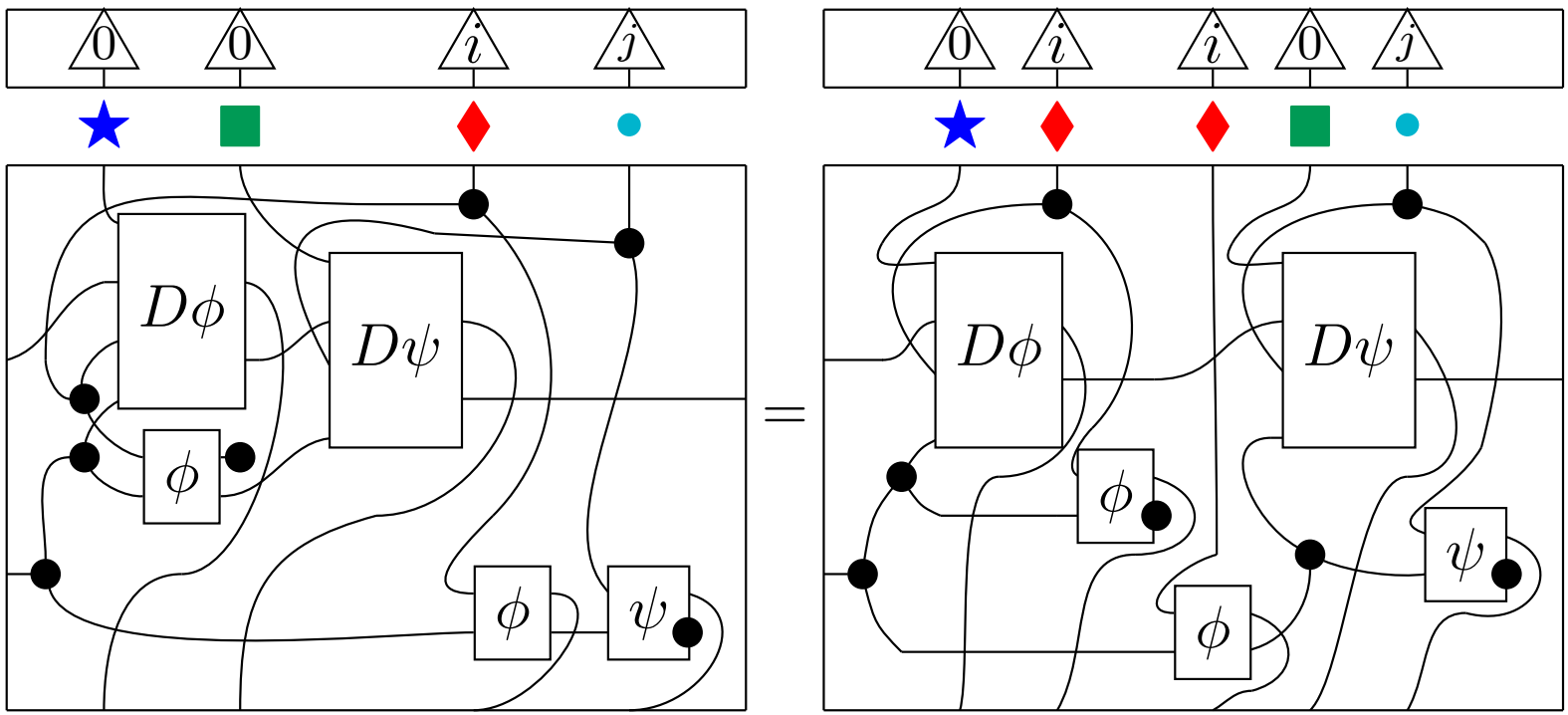

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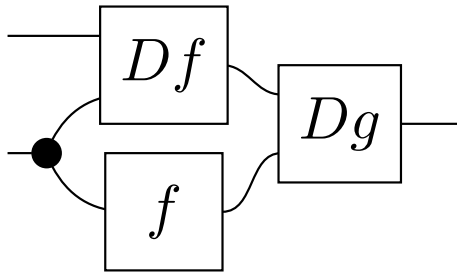

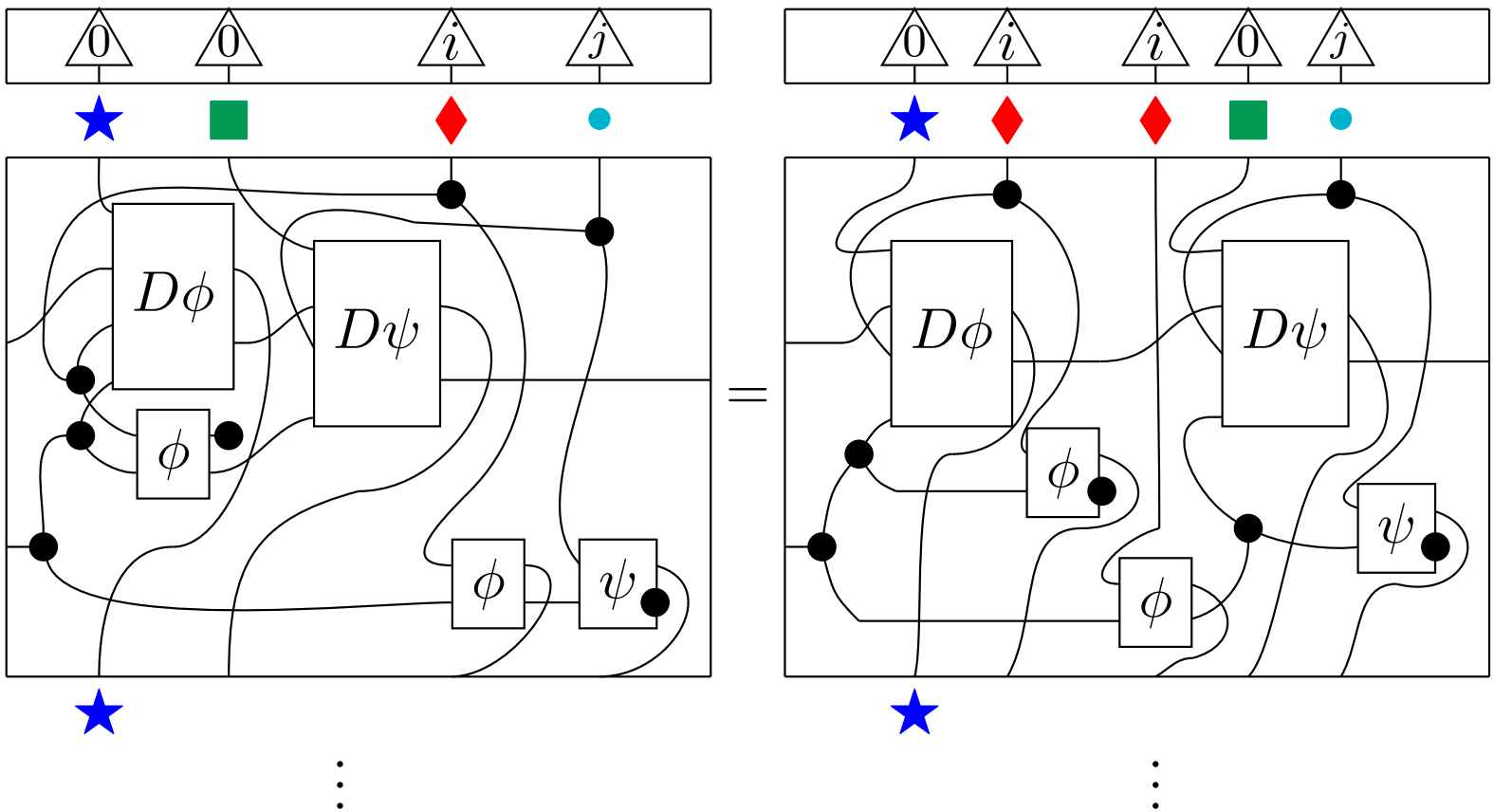

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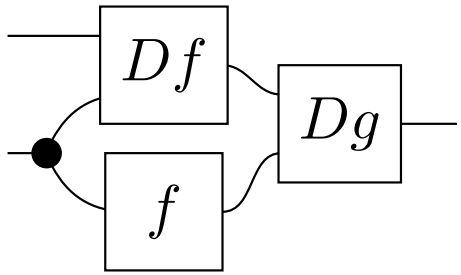

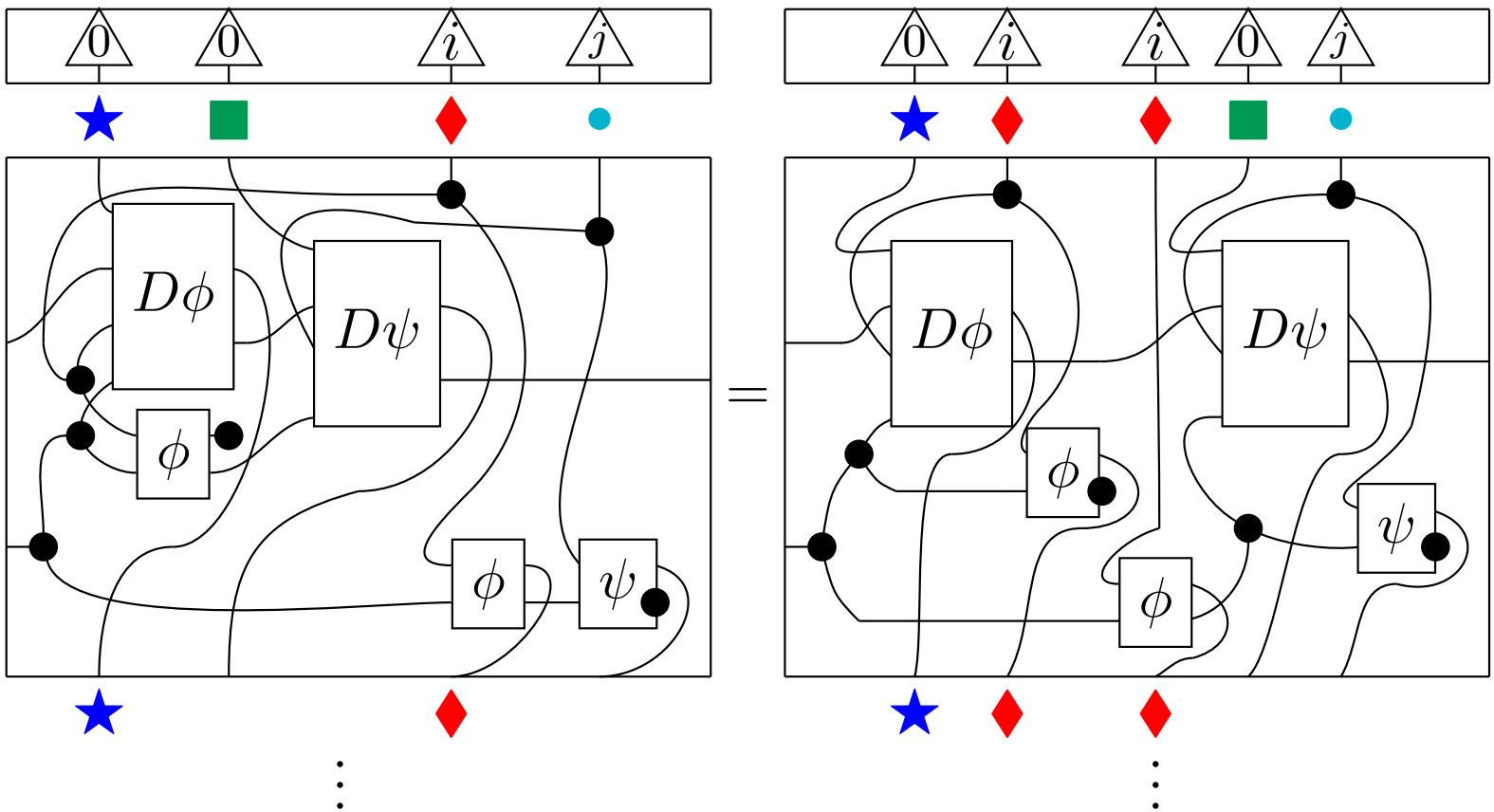

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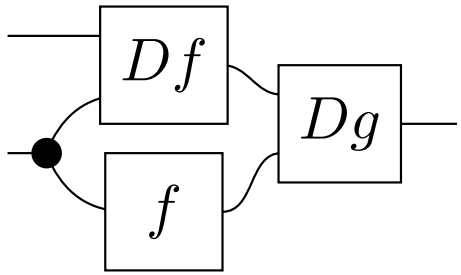

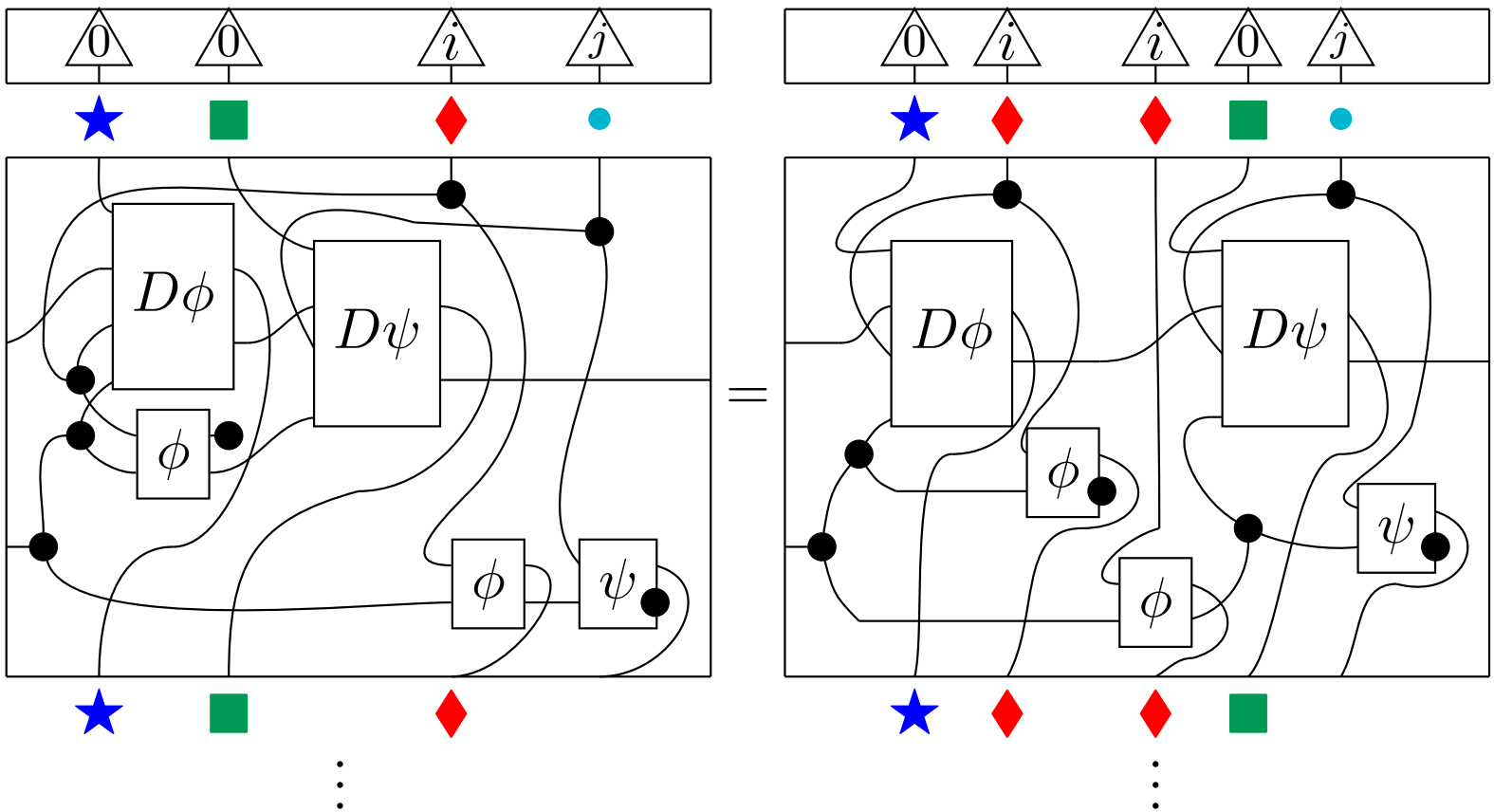

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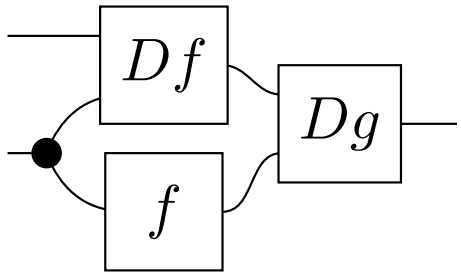
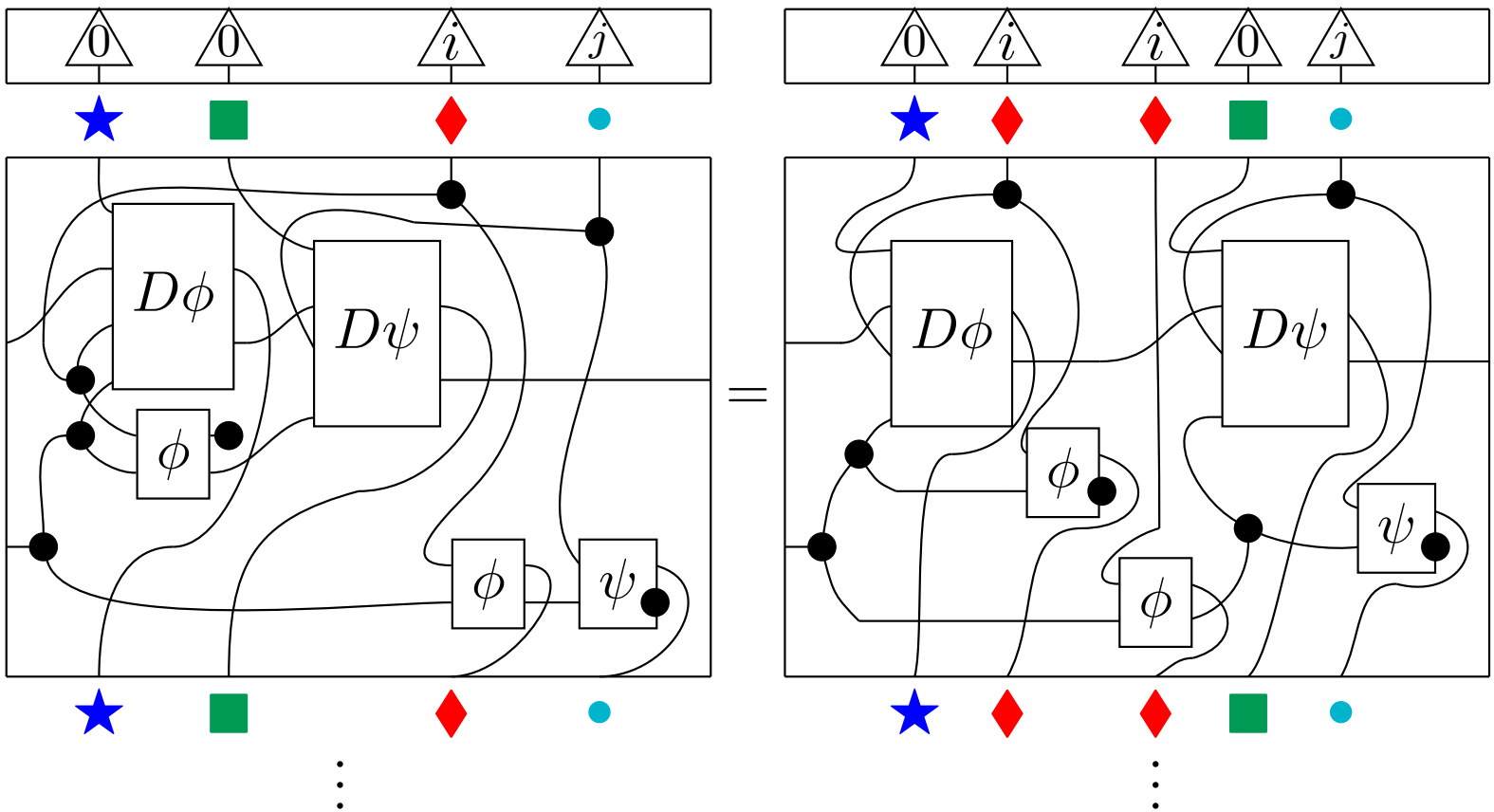
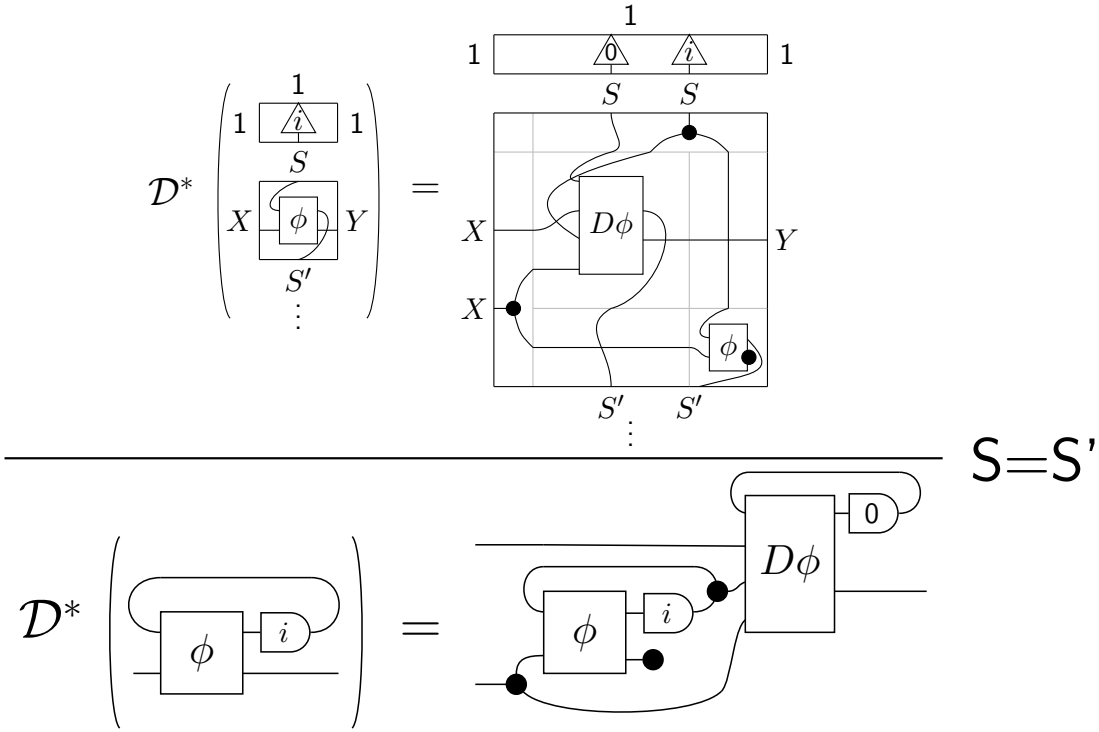




Differentiating circuits



Theorem ($\mathcal{D}^*$ matches BPTT)

The unrolling of $\mathcal{D}^*((i, [\phi]))$ is the component-wise application of D to the unrolling of $(i, [\phi])$.

What if $\phi = \Delta_{\mathbb{R}} \circ \times$?

$$D\left(\times\right) = \quad , \text{ so } \quad D\left(\times\right) =$$

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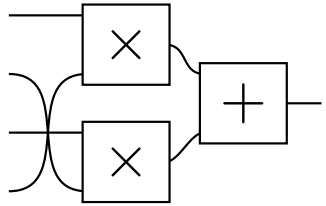
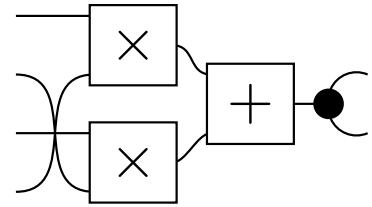
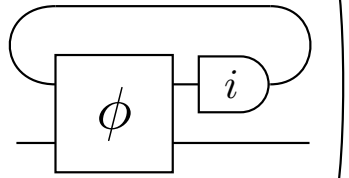
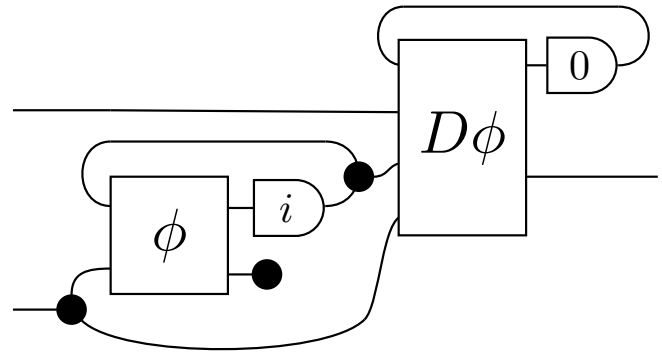
$D\left(\times\right) =$ 

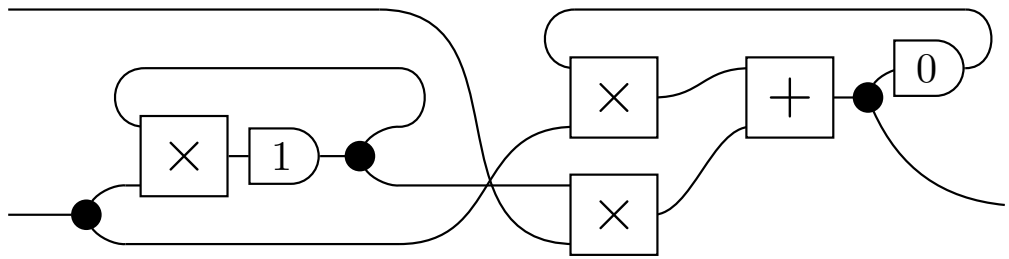
, so $D\left(\times \subset\right) =$ 

Then

$\mathcal{D}^*\left(\right.$ 

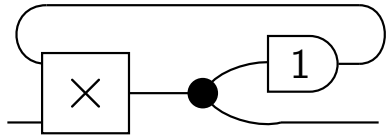
$\left.\right) =$ 

becomes

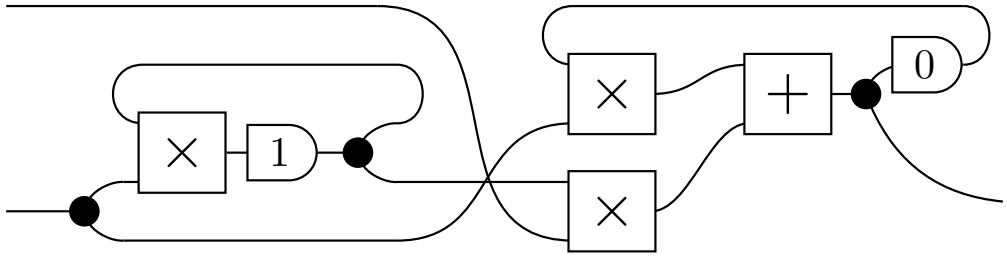


Outline

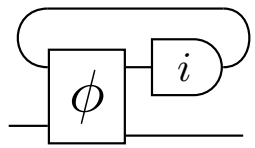
Goals of this talk, again

A. The derivative of 

is this monster



B. There is a general rule for derivatives of stateful functions



C. We understand many properties of this rule.

⋮

Z. ~~Profit??~~ Get paper??

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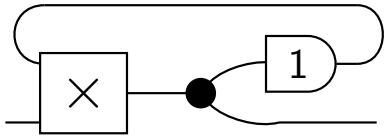
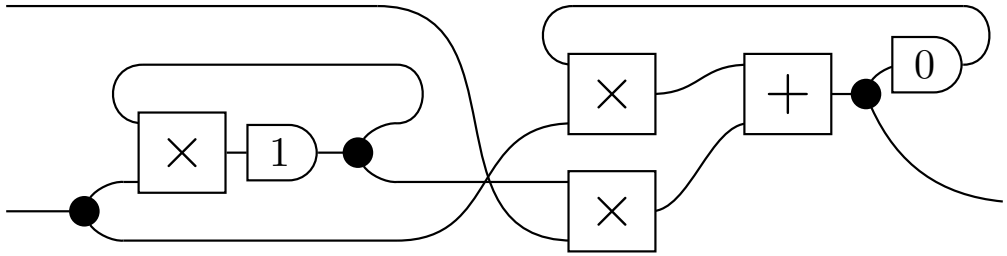
A. The derivative of  is this monster



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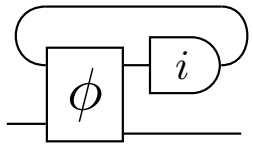

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Future questions (roughly mathematical to practical)

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2. $\mathcal{D}^*$ and derivatives in sequence spaces?
3. Bisimulations and extensional equality?
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11. * Measuring complexity with string diagrams?
12. What happens when $\phi \in \{LSTM, GRU, \ldots\}$?
13. Implementation/plugin to neural net library?

Thanks!